

SEARCH REQUEST FORM

85150

Examiner # (Mandatory): 71618 Requester's Full Name: FRANCISCO C PRATSArt Unit 1651 Location (Bldg/Room#): CM-11A07 Phone (circle 305 306 308) 3665Serial Number: 07/921,188 Results Format Preferred (circle): PAPER DISK E-MAILTitle of Invention PROCESS FOR THE PREPARATION OF CHIRAL ISOFLUORENESInventors (please provide full names): JOHN F. CHIARELLO, BRIAN LEE BUCKWALTER,
TIMOTHY CLAUDE BARDEEarliest Priority Date: 8-3-2000

Keywords (include any known synonyms registry numbers, explanation of initialisms):

"1,4-DIARYL-2-FLUORO-2-BUTENES"
(APPEAR TO BE KNOWN PRODUCTS, DISCLOSED IN U.S. 5,998,673)

ESTERASE

Point of Contact:
Barb O'Brien
Technical Information Specialist
STIC CM1 6A05 308-4291

STRUCTURE SEE CLAIM 6

ELECTED CLAIMS ATTACHED (1-9) (CASE DUE BY
END OF FEB)

Search Topic:

Please write detailed statement of the search topic, and the concept of the invention. Describe as specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples of relevant citations, authors, etc., if known. You may include a copy of the abstract and the broadcast or most relevant claim(s).

- CASE TRANSFERRED TO ME BECAUSE ESTERASE INVOLVED IN
THE SYNTHESIS OF 1,4-DIARYL-2-FLUORO-2 BUTENES

- PLEASE SEARCH ELECTED CLAIMS 1-9 AS FOLLOWS

- CLAIMS 1-5 : SYNTHESIS OF 1,4-DIARYL-2-FLUORO-2
BUTENES W/ ESTERASE

- CLAIM 6-9: COMPOUND (INTERMEDIATES IN SYNTH. OF CLAIMS 1-5
(STRUCTURE SEARCH OF CLAIM 6 IS SUFFICIENT) THANK YOU!

STAFF USE ONLY

Searcher: FORB

Searcher Phone #: _____

Searcher Location: _____

Date Picked Up: _____

Date Completed: 1-28-03Clerical Prep Time: 40Terminal Time: 45

Number of Databases: _____

Type of Search

____ N.A. Sequence

____ A.A. Sequence

4 Structure (#)

____ Bibliographic

____ Litigation 1

____ Fulltext

____ Procurement

____ Other

Vendors (include cost where applicable)

662 STN

____ Questel/Orbit

____ Lexis/Nexis

____ WWW/Internet

____ In-house sequence systems (list)

____ Dialog

____ Dr. Link

____ Westlaw

____ Other (specify)

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=> fil reg; d stat que l14; fil capl; d que nos l16; fil uspatf; d que nos l21

FILE 'REGISTRY' ENTERED AT 11:50:04 ON 28 JAN 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JAN 2003 HIGHEST RN 482277-90-7

DICTIONARY FILE UPDATES: 27 JAN 2003 HIGHEST RN 482277-90-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

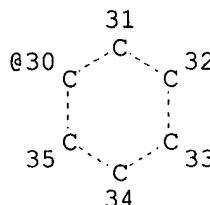
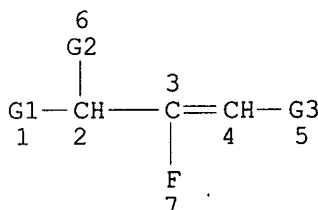
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

L12

STR

Ak @26

Ak-X
@27 28



Ak-Cy
@36 37

VAR G1=30/HY

VAR G2=26/27/CB

VAR G3=30/HY/36

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 26

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L14 23 SEA FILE=REGISTRY SSS FUL L12

100.0% PROCESSED 27046 ITERATIONS

SEARCH TIME: 00.00.02

23 ANSWERS

Formula I from claim 1.
Note that G3 in this drawing = Ar, in claim. Ak-Cy is not supported by the claim, but does appear in the inventors' work, so I included this possibility.

FILE 'CAPLUS' ENTERED AT 11:50:04 ON 28 JAN 2003

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FILE COVERS 1907 - 28 Jan 2003 VOL 138 ISS 5
FILE LAST UPDATED: 27 Jan 2003 (20030127/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L12 STR
L14 23 SEA FILE=REGISTRY SSS FUL L12

~~L16 10 SEA FILE=CAPLUS ABB=ON L14~~ (P)

preparation of these compounds

~~FILE 'USPATFULL'~~ ENTERED AT 11:50:04 ON 28 JAN 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 28 Jan 2003 (20030128/PD)
FILE LAST UPDATED: 28 Jan 2003 (20030128/ED)
HIGHEST GRANTED PATENT NUMBER: US6513163
HIGHEST APPLICATION PUBLICATION NUMBER: US2003019004
CA INDEXING IS CURRENT THROUGH 28 Jan 2003 (20030128/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 28 Jan 2003 (20030128/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2002
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2002

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

L12 STR
L14 23 SEA FILE=REGISTRY SSS FUL L12

~~L21 7 SEA FILE=USPATFULL ABB=ON L14~~ (P)

preparation

~~dup rem 116,121~~

FILE 'CAPLUS' ENTERED AT 11:50:10 ON 28 JAN 2003
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FILE 'USPATFULL' ENTERED AT 11:50:10 ON 28 JAN 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L16
PROCESSING COMPLETED FOR L21

~~L23~~ 15 DUP REM L16 L21 (2 DUPLICATES REMOVED)

ANSWERS '1-10' FROM FILE CAPLUS

ANSWERS '11-15' FROM FILE USPATFULL

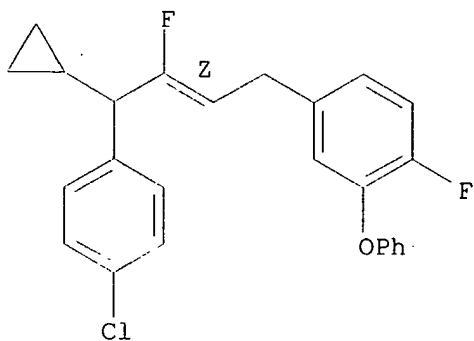
~~=> d ibib abs hitstr l23 1-150 fil cao; d que nos 122~~

L23 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 1
ACCESSION NUMBER: 2001:371701 CAPLUS
DOCUMENT NUMBER: 134:366675
TITLE: Preparation of phenoxyphenylfluorobutenes as
parasiticides
INVENTOR(S): Watson, David Wesley; Heaney, Kathleen; Schwinghammer,
Kurt
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 25 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6235754	B1	20010522	US 1999-235932	19990122

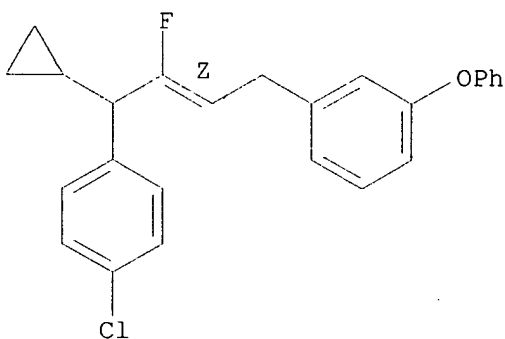
PRIORITY APPLN. INFO.: US 1998-73097P P 19980130
OTHER SOURCE(S): MARPAT 134:366675
AB R3CRR1CF:CR4CHR2R5 [I; R,R1 = H, (halo)(cyclo)alkyl; RR1 = alkylene; R2 =
H, Cl, Br, cyano, OH, alkoxy; R3 = (un)substituted (hetero)aryl; R4 = H or
F; R5 = (un)substituted (phenoxy)phenyl, -biphenyl, -phenoxyphenyl,
etc.] were prepd. Thus, 4-ClC6H4CR:CFCHO (R = cyclopropyl) was condensed
with 4,3-F(PhO)C6H3CH2P(Ph)3Br (prepn. each given) to give, after redn.,
(Z)-4-ClC6H4CHRCF:CHCH2C6H3(OPh)F-3,4 (R as above). Data for biol.
activity of I were given.
IT 200401-86-1P 200401-93-0P 200401-94-1P
200401-95-2P 200401-96-3P 200401-97-4P
200401-98-5P 200402-00-2P 200402-02-4P
200402-03-5P 233760-20-8P 233760-21-9P
340293-60-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except
adverse); BSU (Biological study, unclassified); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(prepn. of phenoxyphenylfluorobutenes as parasiticides)
RN 200401-86-1 CAPLUS
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-
fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



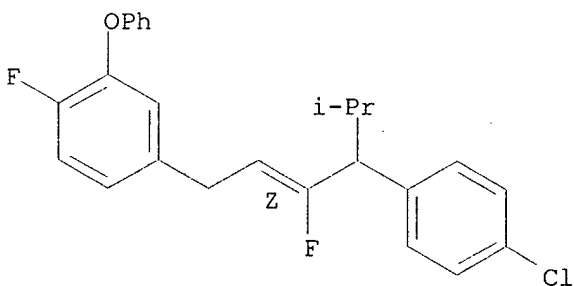
RN 200401-93-0 CAPLUS
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



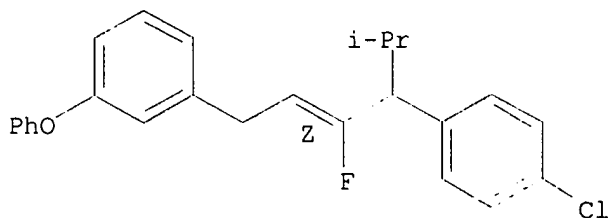
RN 200401-94-1 CAPLUS
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200401-95-2 CAPLUS
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

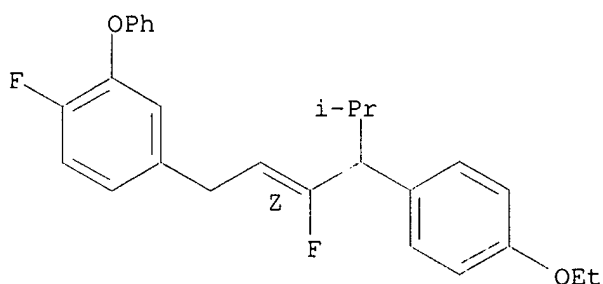
Double bond geometry as shown.



RN 200401-96-3 CAPLUS

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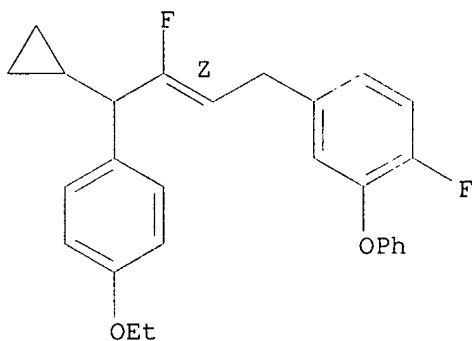
Double bond geometry as shown.



RN 200401-97-4 CAPLUS

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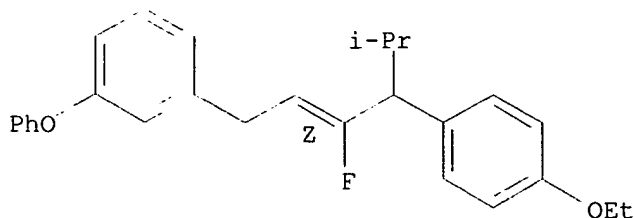
Double bond geometry as shown.



RN 200401-98-5 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

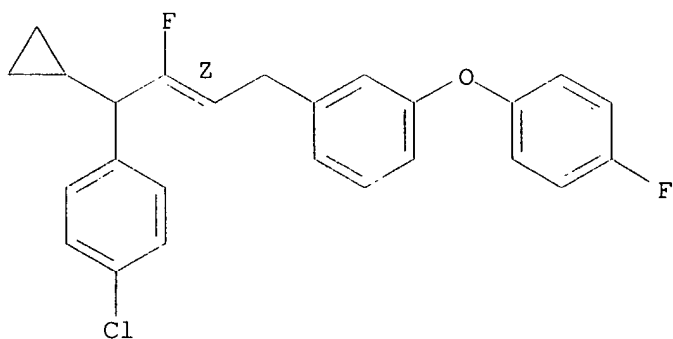
Double bond geometry as shown.



RN 200402-00-2 CAPLUS

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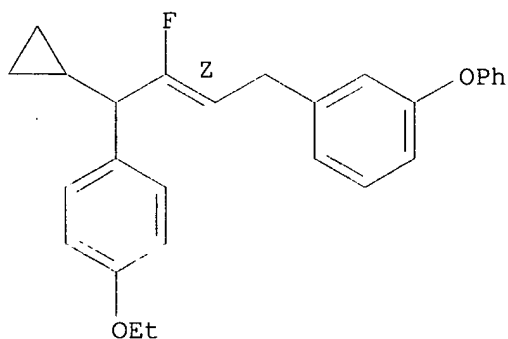
Double bond geometry as shown.



RN 200402-02-4 CAPLUS

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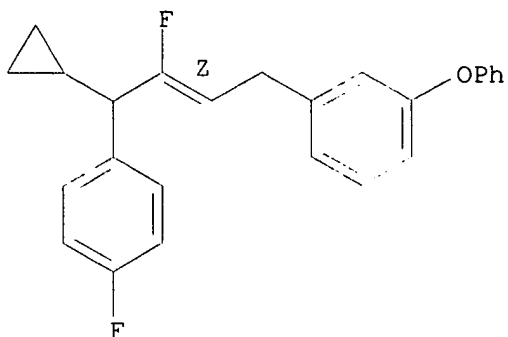
Double bond geometry as shown.



RN 200402-03-5 CAPLUS

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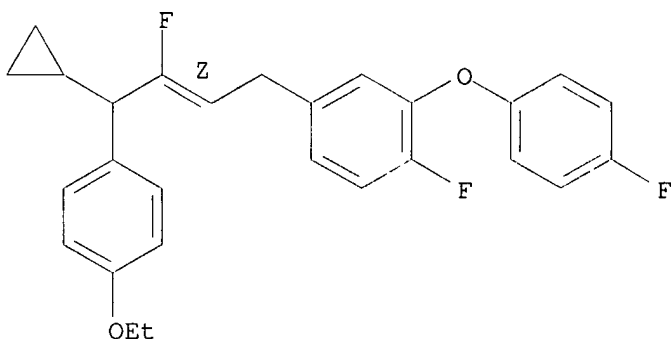
Double bond geometry as shown.



RN 233760-20-8 CAPLUS

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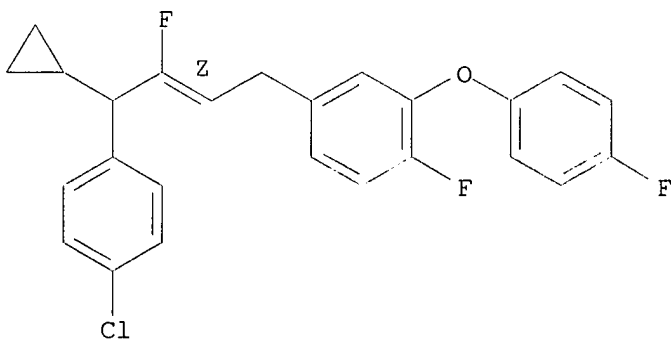
Double bond geometry as shown.



RN 233760-21-9 CAPLUS

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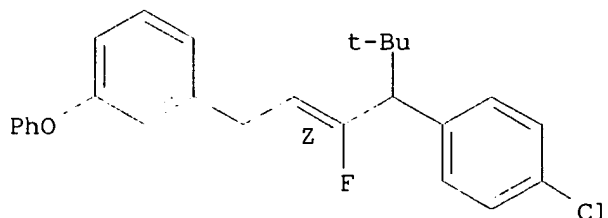
Double bond geometry as shown.



RN 340293-60-9 CAPLUS

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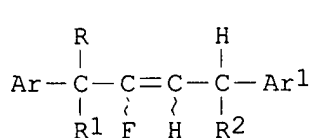
Double bond geometry as shown.



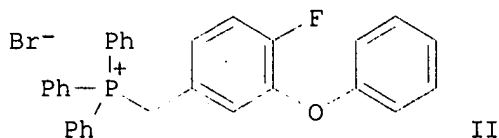
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 2
ACCESSION NUMBER: 1999:780362 CAPLUS
DOCUMENT NUMBER: 132:12197
TITLE: Preparation of 1,4-diaryl-2-fluoro-2-butene derivatives as insecticidal and acaricidal agents
INVENTOR(S): Barnes, Keith D.; Hu, Yulin
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

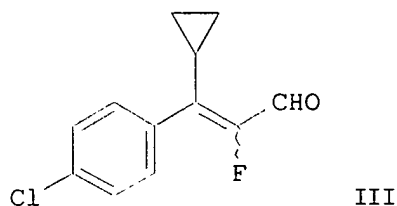
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5998673	A	19991207	US 1997-865244	19970529
PRIORITY APPLN. INFO.:			US 1996-19010P	P 19960603
			US 1997-40461P	P 19970317
OTHER SOURCE(S):		MARPAT 132:12197		
GI				



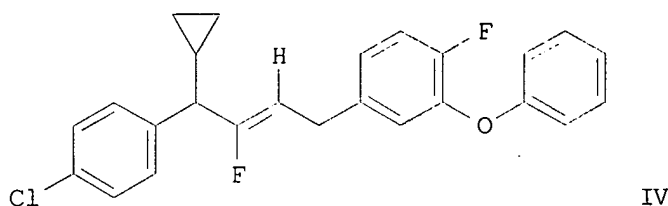
I



II



III



IV

AB Pesticidal 1,4-diaryl-2-fluoro-2-butene compds. I are disclosed, as well as compns. and methods comprising them, for the control of insect and acarid pests [wherein: Ar = (un)substituted Ph, 1- or 2-naphthyl, or a 5- or 6-membered heteroarom. ring; R, R1 = H, alkyl, haloalkyl, cycloalkyl or halocycloalkyl; or R and R1 form a C3-6 cycloalkyl ring optionally substituted halo and/or alkyl; R2 = H, Cl, Br, cyano, or OR3; R3 = H or Cl-4 alkyl; and Ar1 = (un)substituted Ph, biphenyl, pyridyl, 1- or 2-naphthyl, or heteroaryl]. Nineteen example compds. are given. For instance, phosphonium salt II underwent Wittig reaction with aldehyde III (prepn. given), followed by partial redn. of the resultant diene with Mg in MeOH/THF, to give title compd. IV (X = Cl). The analogous compd. IV (X = OEt) gave complete kill of *Spodoptera eridania*, *Diabrotica virgifera*, *Heliothis virescens*, *Aphis fabae*, and *Tetranychus urticae*, at 50-100 ppm.

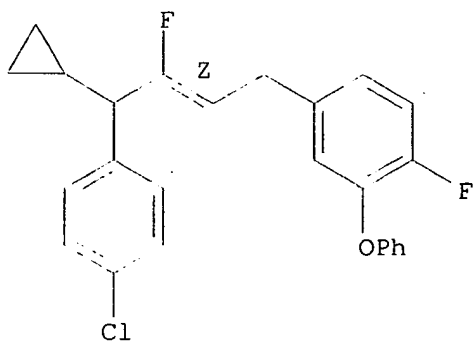
IT 200401-86-1P 200401-93-0P 200401-94-1P
200401-95-2P 200401-96-3P 200401-97-4P
200401-98-5P 200401-99-6P 200402-00-2P
200402-01-3P 200402-02-4P 200402-03-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 1,4-diaryl-2-fluoro-2-butene insecticidal and acaricidal agents)

RN 200401-86-1 CAPLUS

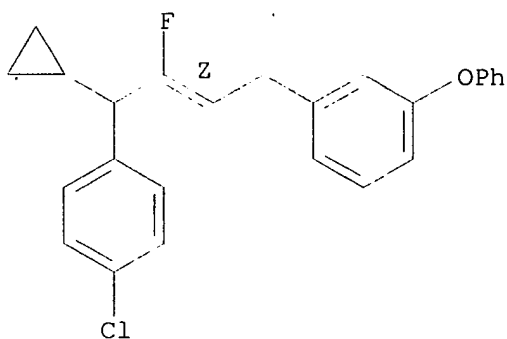
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



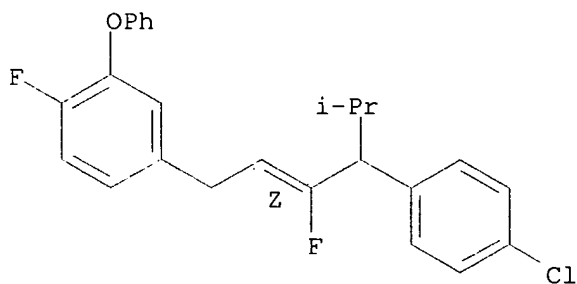
RN 200401-93-0 CAPLUS
 CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



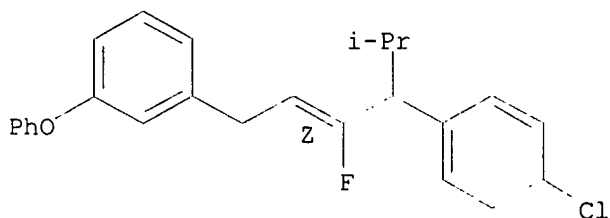
RN 200401-94-1 CAPLUS
 CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



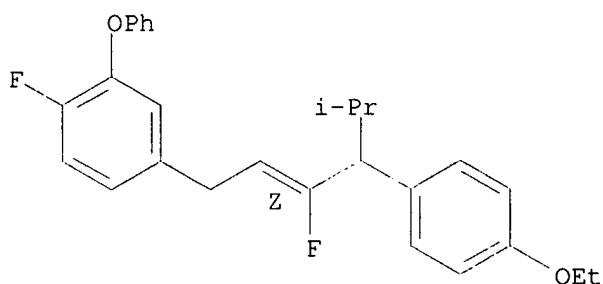
RN 200401-95-2 CAPLUS
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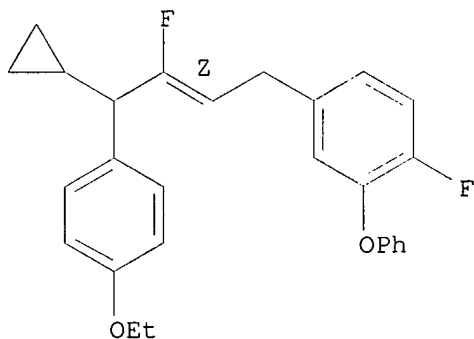
RN 200401-96-3 CAPLUS
CN Benzene, 4-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



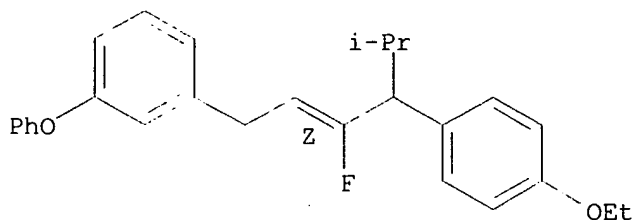
RN 200401-97-4 CAPLUS
CN Benzene, 4-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200401-98-5 CAPLUS
CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

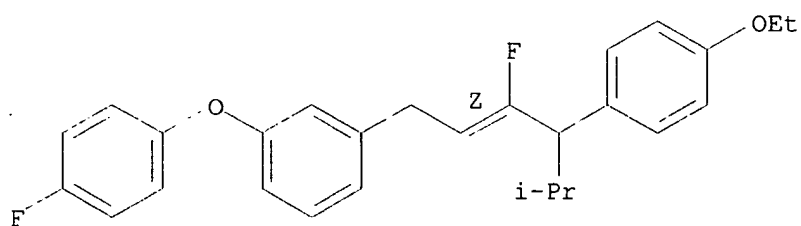
Double bond geometry as shown.



RN 200401-99-6 CAPLUS

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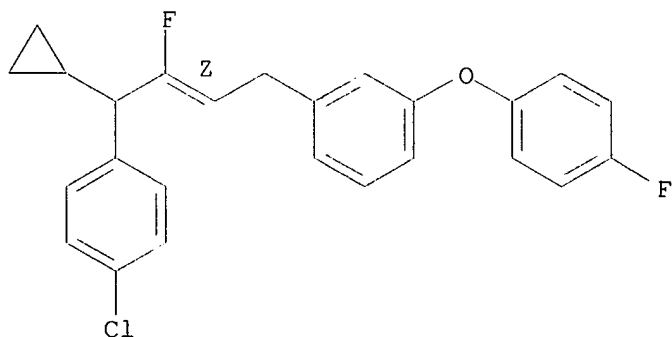
Double bond geometry as shown.



RN 200402-00-2 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

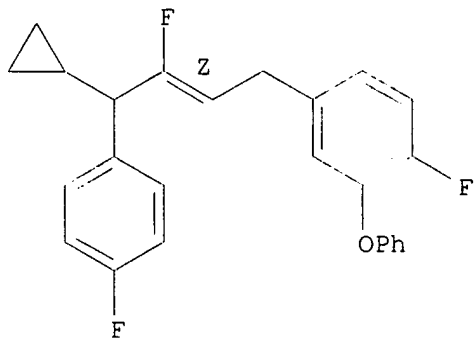
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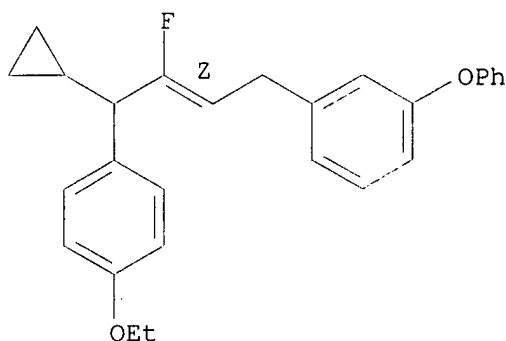
CN Benzene, 4-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



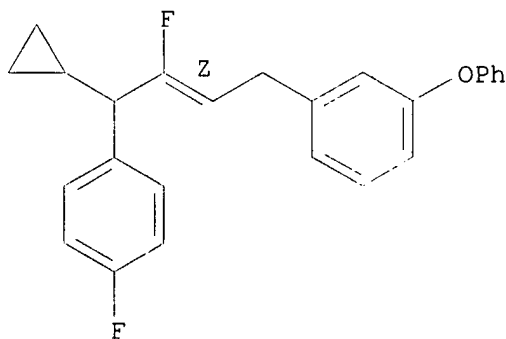
RN 200402-02-4 CAPLUS
CN Benzene, 1-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200402-03-5 CAPLUS
CN Benzene, 1-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:122926 CAPLUS
DOCUMENT NUMBER: 136:183615
TITLE: Process for the preparation of chiral insecticidal and acaricidal 1,4-diaryl-2-fluoro-2-butenes via enzymic

Searched by Barb O'Bryen, STIC 308-4291

hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid methyl ester using esterase

INVENTOR(S): Chiarello, John Francis; Buckwalter, Brian Lee; Barden, Timothy Claude

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012155	A2	20020214	WO 2001-EP9012	20010803
WO 2002012155	A3	20021128		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2002032351	A1	20020314	US 2001-921188	20010802
AU 2001082067	A5	20020218	AU 2001-82067	20010803
PRIORITY APPLN. INFO.:			US 2000-222733P P	20000803
			WO 2001-EP9012 W	20010803

OTHER SOURCE(S): CASREACT 136:183615; MARPAT 136:183615

AB There is provided a process for the prepn. of a chiral compd. of formula $\text{ArC}^*\text{H(R)CF:CHAr1}$ [I; Ar, Ar1 = (un)substituted aryl or a 5- or 6-membered heteroarom. ring; R is C1-4 alkyl, C1-4 haloalkyl, C3-6 cycloalkyl or C3-6 halocycloalkyl; Ar1, is aryl or a 5- or 6-membered heteroarom. ring; C* represents an asym. center] which is useful as an insecticidal and acaricidal agent and for protecting plants from damage caused by insect and acarid attack and infestation (no data). Also provided are intermediate compds. useful in the process of the present invention. This process comprises (a) treating a racemic ester of formula ArCH(R)CO2R4 (II; Ar, R = same as above; R4 = C1-4 alkyl) with an esterase to form a first mixt. of either R-acid of formula ArCH(R)CO2H (III) and S-ester of formula II or of S-acid of formula III and R-ester of formula II, (b) sepg. (R)- or (S)-acid III from said (S)- or (R)-ester II, (c) reducing the chiral acid (R)- or (S)-acid III or (S)- or (R)-ester II to obtain a chiral alc. of formula (R)- or (S)- $\text{ArC}^*\text{H(R)CH2OH}$, (d) transforming the chiral alc. into an ester (R)- or (S)- $\text{ArC}^*\text{H(R)CH2CO2R1}$, (e) fluorinating the latter ester to afford a fluoro-ester (R)- or (S)- $\text{ArC}^*\text{H(R)CHFCO2R1}$, and (f) reacting the latter fluoro-ester with an aldehyde Ar1CH2CHO (Ar1 = same as above) in a solvent in the presence of a base to afford a second mixt. of 4 chiral diastereomeric hydroxy-esters $\text{ArC}^*\text{H(R)CHF(CO2R1)CH(OH)CH2Ar1}$. It further comprises (g) optionally sepg. the second mixt. into a third mixt. each having two chiral diastereomers, (h) treating the hydroxy-ester mixts. with an acylating agent R2COX1 (R2 = C1-4 alkyl; X1 = Cl, Br, R2CO2) to afford a fifth mixt. of 4 chiral diastereomeric acyloxy esters or a seventh mixt. of two chiral diastereomeric acyloxy esters $\text{ArC}^*\text{H(R)CHF(CO2R1)CH(O2CR2)CH2Ar1}$, (i) optionally sepg. the sixth or seventh mixt. not essentially pure chiral diastereomeric acyloxy ester, (j) hydrolyzing the pure acyloxy esters or mixts. of esters to afford a hydroxy acid $\text{ArC}^*\text{H(R)CHF(CO2H)CH(OH)CH2Ar1}$, and (k) heating the hydroxy acid with a arylsulfonyl halide to afford I. Thus, Me (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate was treated with horse liver esterase in water (pH 7.5) to give 37.9% (2R)-(4-chlorophenyl)(cyclopropyl)ethanoic acid and 36.2% Me (2S)-(4-

chlorophenyl)(cyclopropyl)ethanoate, each of which was reduced by BH3.THF/THF at room temp. for 4 h and DIBAL/CH2Cl2 warming from -78.degree. to room temp. and at room temp. for 1 h, resp., to give 84% (2R)-(4-chlorophenyl)(cyclopropyl)ethanol and 80% (2S)-(4-chlorophenyl)(cyclopropyl)ethanol, resp. Each of (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethanol was tosylated by tosyl chloride in the presence of Et3N in CH2Cl2 to (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethyl p-toluenesulfonate, resp., which underwent cyanation with NaCN in DMSO at 90.degree. for 3 h to give (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile, resp. Alkali hydrolysis of (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile in a mixt. of 10% aq. NaOH and methanol under reflux for 18 h followed by acidification with concd. HCl gave (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoic acid, resp., which was esterified with MeOH in the presence of HCl at room temp. for 18 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate, resp. Lithiation of the each ester with lithium diisopropylamide (LDA) in THF at -78.degree. to 0.degree. followed by fluorination with (PhSO2)2NF at -78.degree. to room temp. and room temp. for 2 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate, resp. Lithiation of Me (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate with LDA in THF at -78.degree. for 15 min followed by addn. reaction with 4-fluoro-3-phenoxyphenylacetaldehyde at -78.degree. for 2 h gave, after silica gel chromatog., an oil (A) contg. (2R,3R) and (2R,3S) or (2S,3R) or (2R,3S)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate and an oil contg. (2S,3S) and (2S,3R) or (2R,3S)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate (steps f and g). Acetylation of the oil A with Ac2O in the presence of DAMP in CH2Cl2 at room temp. for 2 h gave Me (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate and Me (2R,3S or 2S,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate (step h and i). Alkali hydrolysis of the latter diastereomer in a mixt. of 10% aq. NaOH, MeOH, and THF under reflux for 1 h gave (2S,3R or 2R,3S)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid (step j) which was heated with tosyl chloride in collidine at 170.degree. for 2 h to give 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene as a colorless oil (step k).

IT **398453-72-0P**, 4-[(2Z,4S)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene **398453-73-1P**, 4-[(2E,4S)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene **398453-74-2P**, 4-[(2E,4R)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene **398453-75-3P**, 4-[(2Z,4R)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

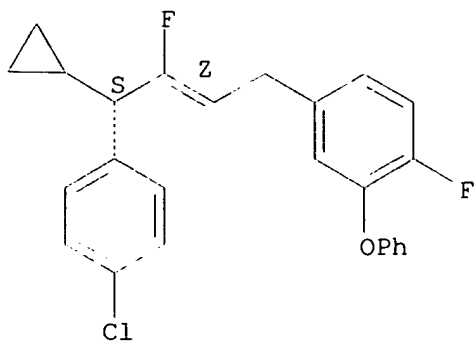
(process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

RN 398453-72-0 CAPLUS

CN Benzene, 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

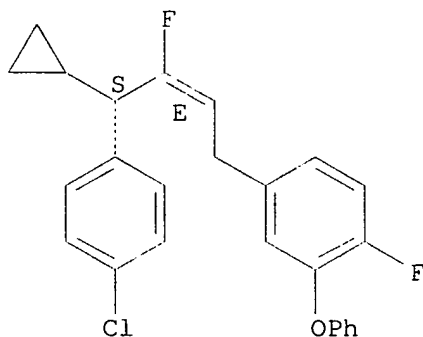
Absolute stereochemistry.

Double bond geometry as shown.



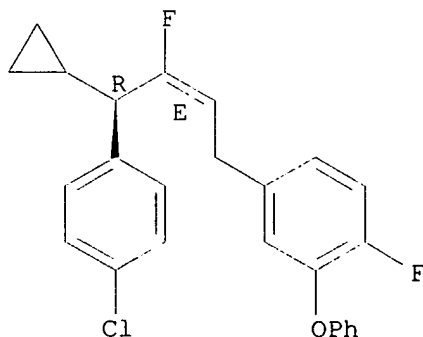
RN 398453-73-1 CAPLUS
CN Benzene, 4-[(2E,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



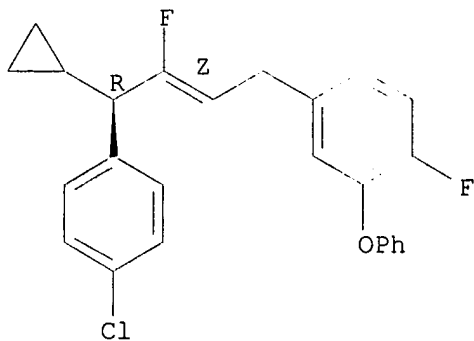
RN 398453-74-2 CAPLUS
CN Benzene, 4-[(2E,4R)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 398453-75-3 CAPLUS
CN Benzene, 4-[(2Z,4R)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L23 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:816615 CAPLUS

DOCUMENT NUMBER: 135:344285

TITLE: 1,4-Diaryl-2-fluoro-4-cyano-2-butenes, process for their preparation and useful intermediates

INVENTOR(S): Hu, Yulin; Hunt, David Allen

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

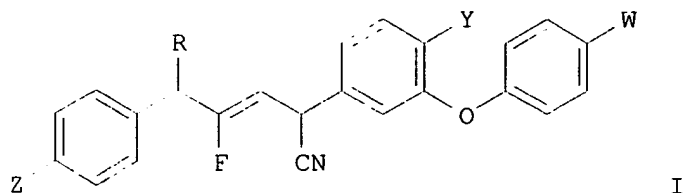
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001083428	A1	20011108	WO 2001-EP4958	20010503
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002019556	A1	20020214	US 2001-849298	20010504
US 6444838	B2	20020903		

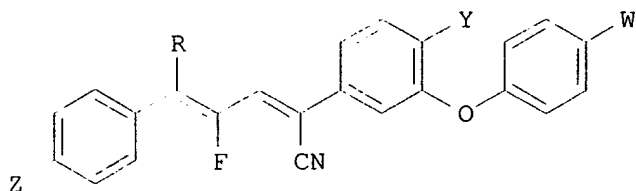
PRIORITY APPLN. INFO.: US 2000-201826P P 20000504

OTHER SOURCE(S): CASREACT 135:344285; MARPAT 135:344285

GI



I



II

AB The prepn. and intermediates useful in the prepn. of 1,4-diaryl-2-fluoro-4-cyano-2-butene compds. [ArCH(R)CF=CHCH(CN)Ar'] are described. Particularly preferred are compds. of formula I and II (Z = Cl, F, OEt; R = *c*-C₃H₅, *i*Pr; W and Y are independently H or F). Compds. II are converted into I in refluxing MeOH/THF with added magnesium under nitrogen.

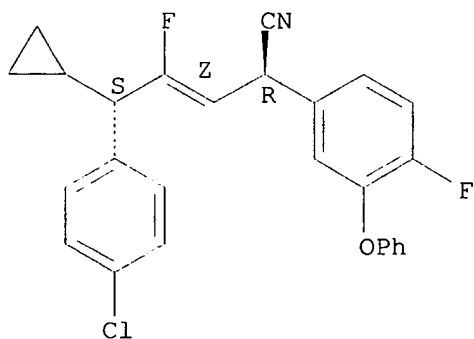
IT 371759-00-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 371759-00-1 CAPLUS

CN Benzeneacetonitrile, .alpha.-[(1Z,3R)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoro-1-propenyl]-4-fluoro-3-phenoxy-, (.alpha.S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:137168 CAPLUS

DOCUMENT NUMBER: 134:178341

TITLE: Preparation of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes.

INVENTOR(S): Hu, Yulin; Hunt, David Allen; Liu, Weiguo

PATENT ASSIGNEE(S): American Cyanamid Company, USA

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

Searched by Barb O'Bryen, STIC 308-4291

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001012578	A1	20010222	WO 2000-US21464	20000807
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6291721	B1	20010918	US 1999-373262	19990812
BR 2000013100	A	20020430	BR 2000-13100	20000807
EP 1202948	A1	20020508	EP 2000-952575	20000807
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			

PRIORITY APPLN. INFO.: US 1999-373262 A 19990812
WO 2000-US21464 W 20000807

OTHER SOURCE(S): CASREACT 134:178341; MARPAT 134:178341

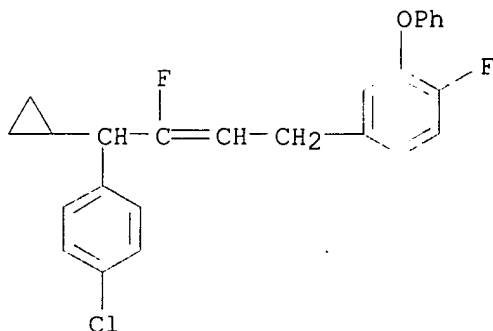
AB Ar(R)C:CHOR [R = H, alkyl, haloalkyl, cycloalkyl, halocycloalkyl; R1 = alkyl; Ar = (substituted) Ph, naphthyl, heteroaryl], were prepd. in the absence of phosphonium halides by reaction of ArCHRCHO (variables as above) with R1OH in the presence of acid, or reaction of ArCHRCH(OR)2 in an aprotic solvent at elevated temp. in the presence of acid. Thus, 1-[1-(p-chlorophenyl)-2,2-dimethoxyethyl]cyclopropane (prepn. given) was refluxed with 4-MeC6H4SO3H in PhMe with distn. of PhMe/MeOH to give 96% 1-[1-(p-chlorophenyl)-2-methoxyvinyl]cyclopropane. This in H2O contg. KOH and 18-crown-6 at 7-10.degree. was treated with CHCl2F followed by stirring for 36 h at 10-13.degree., addn. of H2O, and heating at 70-75.degree. for 4 h to give (Z)- and (E)-p-chloro-.beta.-cyclopropyl-.alpha.-fluorocinnamaldehyde as a separable mixt. This was used to prep. (Z)-1-[1-(p-chlorophenyl)-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-2-butenyl]cyclopropane.

IT 269398-40-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes)

RN 269398-40-5 CAPLUS

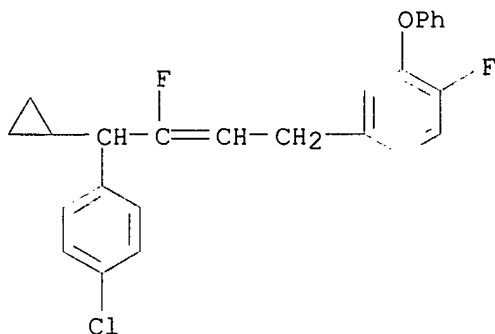
CN Benzene, 4-[4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)



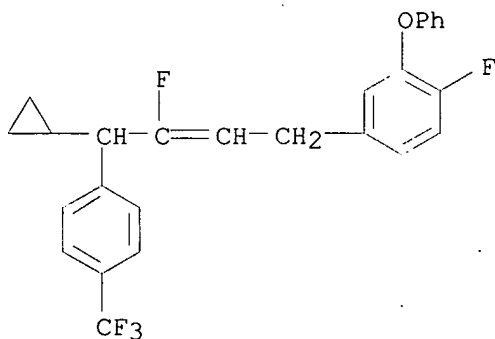
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:351483 CAPLUS
DOCUMENT NUMBER: 132:347408
TITLE: 1,4-Diaryl-2-fluoro-1-buten-3-ol compounds and their
use in the preparation of 1,4-diaryl-2-fluoro-1,3-
butadiene and 1,4-diaryl-2-fluoro-2-butene compounds
INVENTOR(S): Hu, Yulin; Hunt, David Allen
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000029362	A1	20000525	WO 1999-US26434	19991109
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 9915368	A	20010814	BR 1999-15368	19991109
EP 1131273	A1	20010912	EP 1999-958849	19991109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002529524	T2	20020910	JP 2000-582353	19991109
US 6342642	B1	20020129	US 2001-856229	20010813
PRIORITY APPLN. INFO.: US 1998-192680 A 19981116 WO 1999-US26434 W 19991109				
OTHER SOURCE(S): MARPAT 132:347408				
AB	Prepn. of 1,4-diaryl-2-fluoro-1-buten-3-ol compds. ArCR:CFCH(OH)CH2Ar1 [R = H, alkyl, haloalkyl, cycloalkyl; Ar = (un)substituted Ph; Ar1 = (un)substituted Ph, phenoxyphenyl, biphenyl, etc.] and the use of these compds. in the prepn. of 1,4-diaryl-2-fluoro-1,3-butadiene compds. ArCR:CFCH:CHAr1 and 1,4-diaryl-2-fluoro-2-butene compds. ArCHRCF:CHCH2Ar1 are given. E.g., treating 1-(p-chlorophenyl)-1-cyclopropyl-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-1-buten-3-ol (prepn. given) with NaH/p-toluenesulfonyl chloride gave 61% 1-(p-chlorophenyl)-1-cyclopropyl-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-1,3-butadiene.			
IT	269398-40-5P 269398-41-6P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of diarylfluorobutenol compds. and their use in the prepn. of butadiene and butene derivs.)			
RN	269398-40-5 CAPLUS			
CN	Benzene, 4-[4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)			



RN 269398-41-6 CAPLUS
CN Benzene, 4-[4-cyclopropyl-3-fluoro-4-[4-(trifluoromethyl)phenyl]-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:505746 CAPLUS
DOCUMENT NUMBER: 131:126722
TITLE: Preparation of diarylfluorobutene derivatives as ectoparasiticides and anthelmintics
INVENTOR(S): Watson, David Wesley; Heaney, Kathleen; Schwinghammer, Kurt Allen
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: Eur. Pat. Appl., \20363 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 933027	A1	19990804	EP 1999-300544	19990126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 11255605	A2	19990921	JP 1999-15636	19990125
ZA 9900692	A	20000728	ZA 1999-692	19990128
BR 9901066	A	20010424	BR 1999-1066	19990128
AU 9914257	A1	19990819	AU 1999-14257	19990129
CN 1236612	A	19991201	CN 1999-101729	19990129
PRIORITY APPLN. INFO.:			US 1998-15258	A 19980130

OTHER SOURCE(S): MARPAT 131:126722

AB The invention relates to methods and compns. for controlling, preventing and protecting animals and humans from infestation and infection by arthropod and helminth parasites, by administering or applying 1,4-diaryl-2-fluoro-2-butene or 1,4-diaryl-2,3-difluoro-2-butene derivs. ArCRR1CF:CZCHAR1R2 [Ar = (un)substituted Ph, naphthyl or heteroaryl; R, R1 = H or (un)substituted (halo)alkyl or (halo)cycloalkyl; RCR1 = (un)substituted cycloalkyl; Z = H or F; R2 = H, Cl, Br, CN, OH or alkoxy; Ar1 = (un)substituted phenoxyphenyl] or their (Z)- or (E)-isomers. Prepn. of the compds. is given.

IT 200401-86-1P 200401-93-0P 200401-94-1P
200401-95-2P 200401-96-3P 200401-97-4P
200401-98-5P 200401-99-6P 200402-00-2P
200402-02-4P 200402-03-5P 233760-20-8P
233760-21-9P

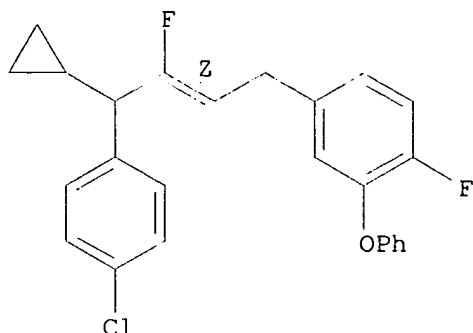
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. as ectoparasiticide and anthelmintic)

RN 200401-86-1 CAPLUS

CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

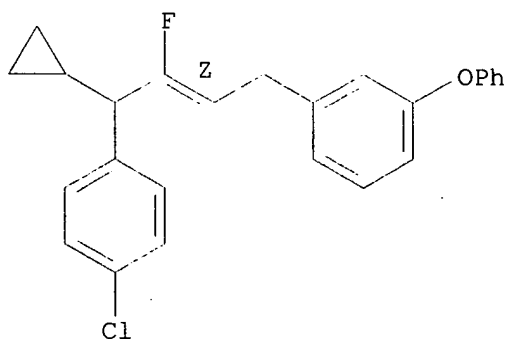
Double bond geometry as shown.



RN 200401-93-0 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

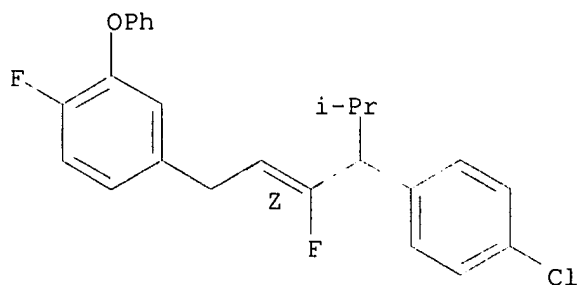
Double bond geometry as shown.



RN 200401-94-1 CAPLUS

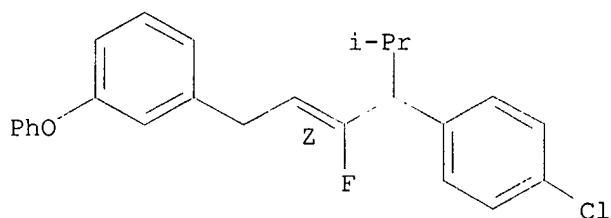
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



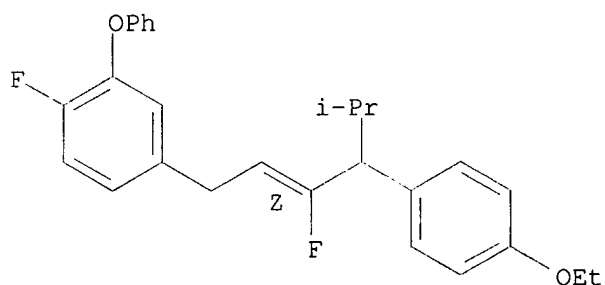
RN 200401-95-2 CAPLUS
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



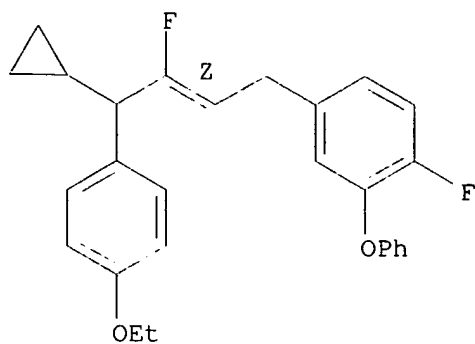
RN 200401-96-3 CAPLUS
CN Benzene, 4-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-
2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200401-97-4 CAPLUS
CN Benzene, 4-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-1-
fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

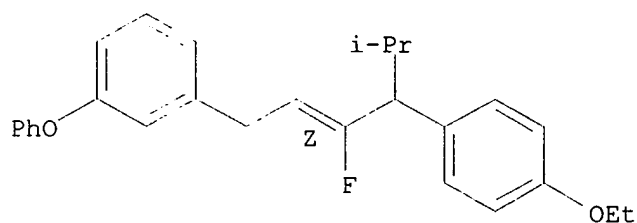
Double bond geometry as shown.



RN 200401-98-5 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy-
(9CI) (CA INDEX NAME)

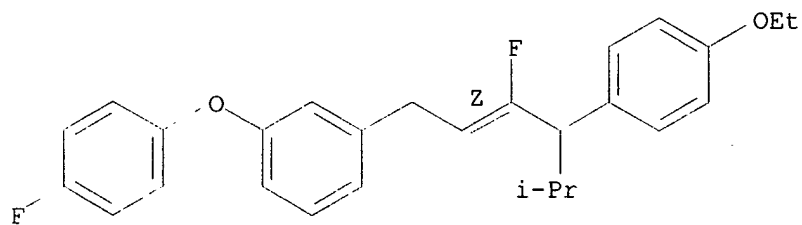
Double bond geometry as shown.



RN 200401-99-6 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-(4-
fluorophenoxy)- (9CI) (CA INDEX NAME)

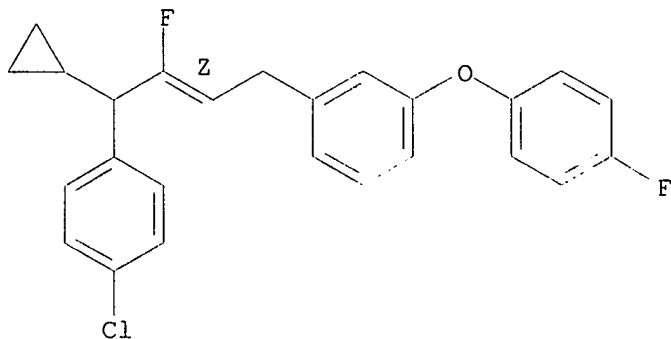
Double bond geometry as shown.



RN 200402-00-2 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-(4-
fluorophenoxy)- (9CI) (CA INDEX NAME)

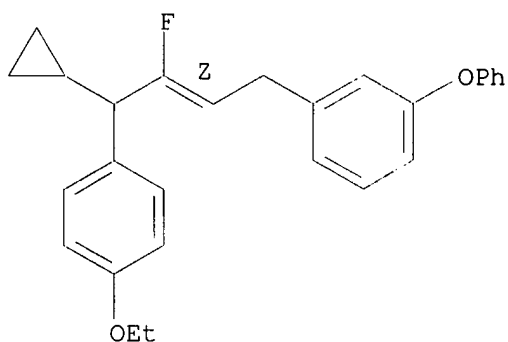
Double bond geometry as shown.



RN 200402-02-4 CAPLUS

CN Benzene, 1-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

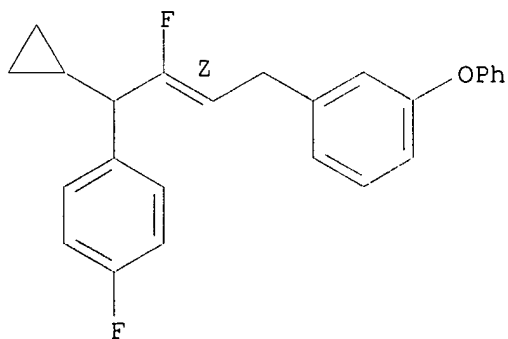
Double bond geometry as shown.



RN 200402-03-5 CAPLUS

CN Benzene, 1-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

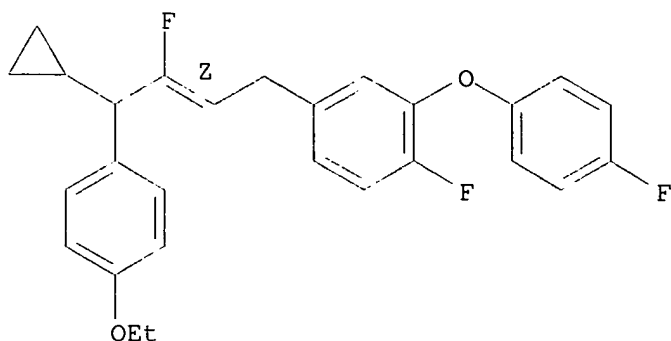
Double bond geometry as shown.



RN 233760-20-8 CAPLUS

CN Benzene, 4-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-1-fluoro-2-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

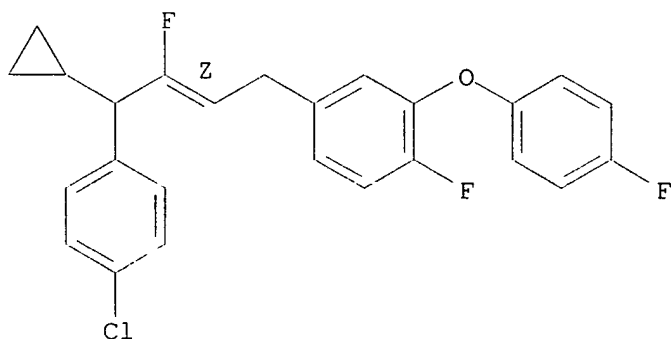
Double bond geometry as shown.



RN 233760-21-9 CAPLUS

CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:801906 CAPLUS

DOCUMENT NUMBER: 128:61344

TITLE: Preparation of 1,4-diaryl-2-fluoro-2-butene insecticidal and acaricidal agents

INVENTOR(S): Barnes, Keith Douglas; Hu, Yulin

PATENT ASSIGNEE(S): American Cyanamid Company, USA

SOURCE: Eur. Pat. Appl., 41 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

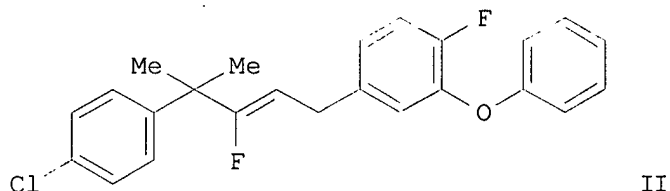
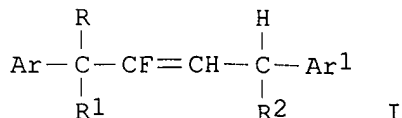
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 811593	A1	19971210	EP 1997-303657	19970529
EP 811593	B1	20020724		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 5849958	A	19981215	US 1997-819623	19970317
CN 1167105	A	19971210	CN 1997-105522	19970529
JP 10072385	A2	19980317	JP 1997-154272	19970529
AT 221037	E	20020815	AT 1997-303657	19970529
CA 2206585	AA	19971203	CA 1997-2206585	19970530

NO 9702502	A	19971204	NO 1997-2502	19970602
AU 9724640	A1	19971211	AU 1997-24640	19970602
AU 729500	B2	20010201		
BR 9703426	A	19980915	BR 1997-3426	19970602
ZA 9704845	A	19981202	ZA 1997-4845	19970602
PRIORITY APPLN. INFO.:			US 1996-660221	A 19960603
			US 1997-819623	A 19970317
OTHER SOURCE(S):		MARPAT 128:61344		
GI				



AB The title compds. [I; Ar = (un)substituted Ph; 1- or 2-naphthyl, 5-6 membered heteroaryl; R, R1 = H, C1-4 alkyl, C1-4 haloalkyl, etc.; R2 = H, Cl, Br, CN, OR3; R3 = H, C1-4 alkyl; Ar1 = (un)substituted phenoxyphenyl], useful for the control of insect and acarid pests, were prepd. Thus, reaction of (Z)-1-bromo-4-(p-chlorophenyl)-3-fluoro-4-methyl-2-pentene with 4-fluoro-3-phenoxybenzeneboronic acid in the presence of Pd(dba)₂ and K₂CO₃ in PhMe/EtOH afforded 86% (Z)-II which showed 100% control against, e.g., southern armyworm and western corn rootworm.

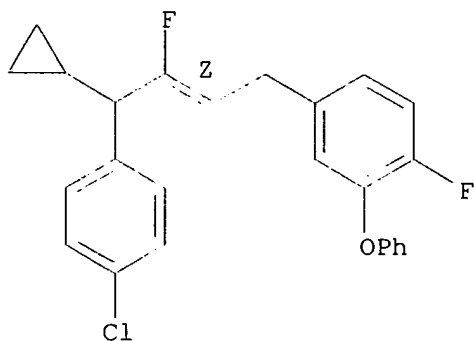
IT 200401-86-1P 200401-93-0P 200401-94-1P
200401-95-2P 200401-96-3P 200401-97-4P
200401-98-5P 200401-99-6P 200402-00-2P
200402-01-3P 200402-02-4P 200402-03-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 1,4-diaryl-2-fluoro-2-butene insecticidal and acaricidal agents)

RN 200401-86-1 CAPLUS

CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

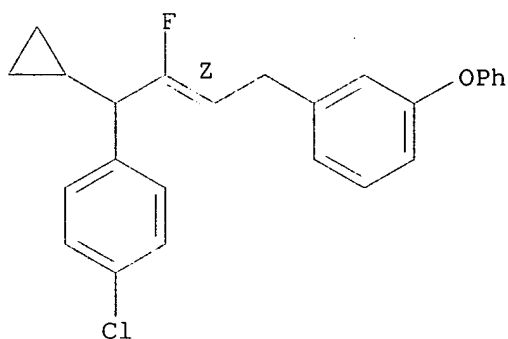
Double bond geometry as shown.



RN 200401-93-0 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

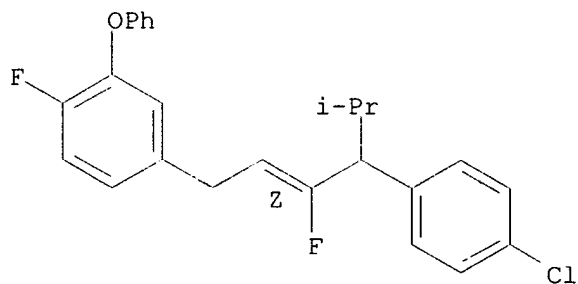
Double bond geometry as shown.



RN 200401-94-1 CAPLUS

CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

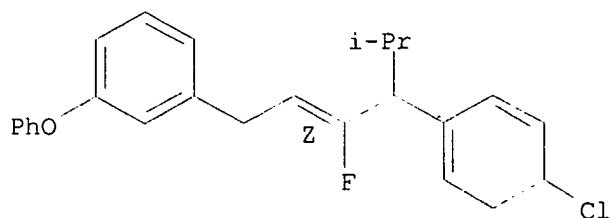
Double bond geometry as shown.



RN 200401-95-2 CAPLUS

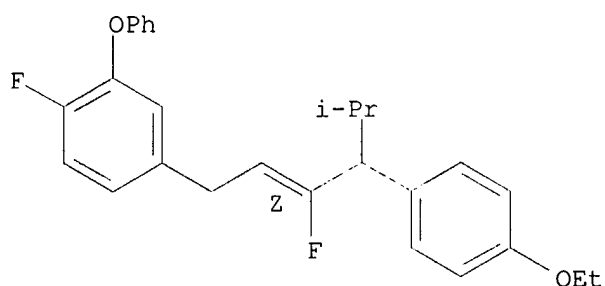
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



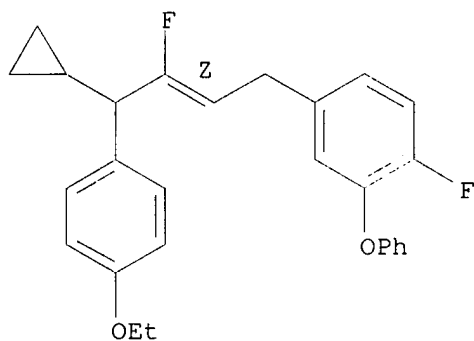
RN 200401-96-3 CAPLUS
CN Benzene, 4-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



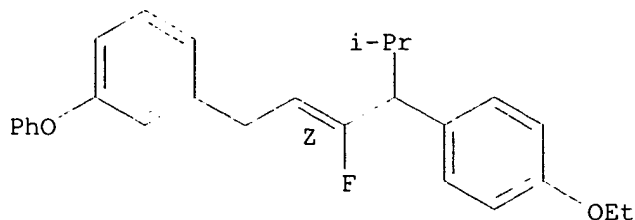
RN 200401-97-4 CAPLUS
CN Benzene, 4-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200401-98-5 CAPLUS
CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

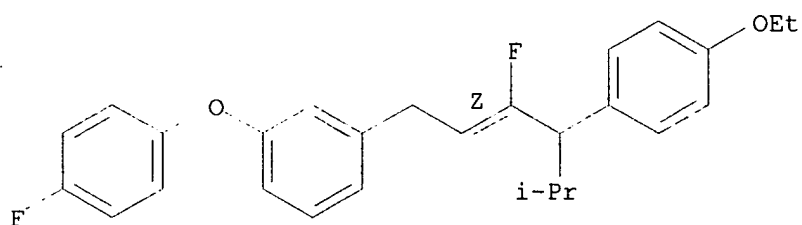
Double bond geometry as shown.



RN 200401-99-6 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

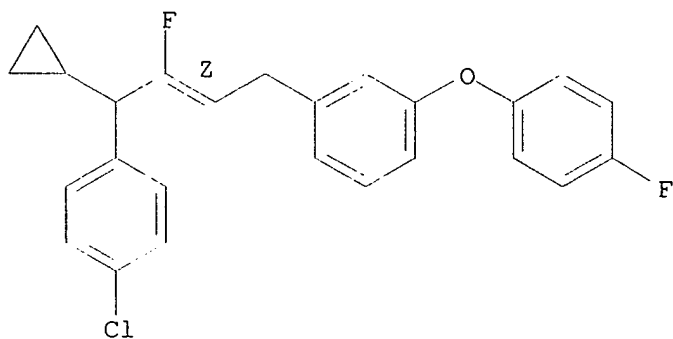
Double bond geometry as shown.



RN 200402-00-2 CAPLUS

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

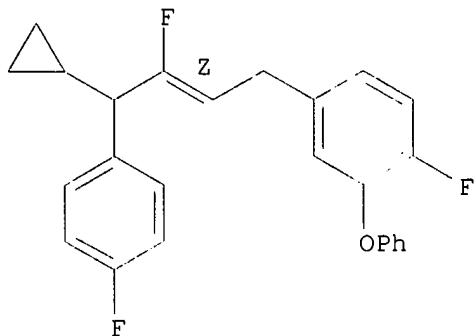
Double bond geometry as shown.



RN 200402-01-3 CAPLUS

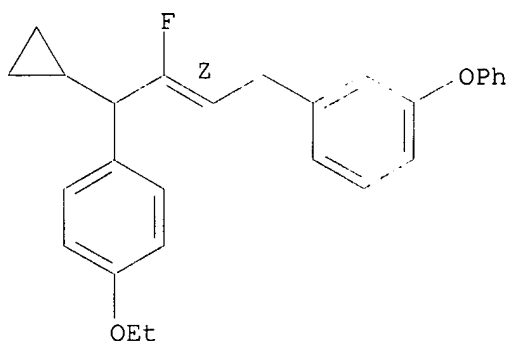
CN Benzene, 4-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



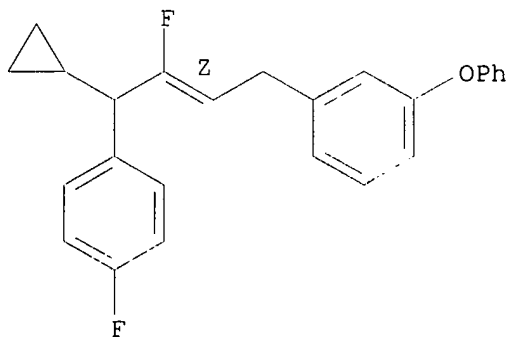
RN 200402-02-4 CAPLUS
CN Benzene, 1-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200402-03-5 CAPLUS
CN Benzene, 1-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

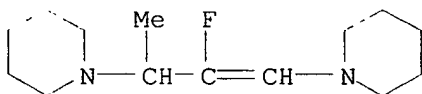
Double bond geometry as shown.



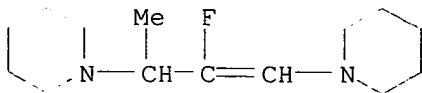
L23 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:47394 CAPLUS
DOCUMENT NUMBER: 128:140757
TITLE: Nucleophilic addition of trimethylsilylamines to
2-halo-2-alkenals
AUTHOR(S): Rulev, A. Yu.; Kuznetsova, T. A.; Mokov, A. S.;
Sherstyannikova, L. V.; Keiko, N. A.; Voronkov, M. G.

Searched by Barb O'Bryen, STIC 308-4291

CORPORATE SOURCE: Siberian Division, Institute of Organic Chemistry,
Russian Academy of Sciences, Irkutsk, 664033, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of
Zhurnal Organicheskoi Khimii) (1997), 33(1), 26-28
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2-Halo-2-alkenals react with trimethylsilyl derivs. of secondary amines to
give the products of 1,2-and 1,4-addn. Both the structure of the starting
aldehyde and the nature of the substituent at the N atom are responsible
for reaction selectivity.
IT 176374-20-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 176374-20-2 CAPLUS
CN Piperidine, 1,1'-(2-fluoro-3-methyl-1-propene-1,3-diyl)bis- (9CI) (CA
INDEX NAME)



L23 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:134963 CAPLUS
DOCUMENT NUMBER: 124:316943
TITLE: Reactions of .alpha.-halo .alpha.,.beta.-unsaturated
aldehydes with secondary amines
AUTHOR(S): Rulev, A. Yu.; Keiko, N. A.; Voronkov, M. G.
CORPORATE SOURCE: Irkutsk Inst. Org. Chem., Irkutsk, 664033, Russia
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1996),
(1), 135-8
CODEN: IASKEA
PUBLISHER: Institut Organicheskoi Khimii im. N. D. Zelinskogo
Rossiiskoi Akademii Nauk
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Reactions of 2-halo-2-alkenals R2R1C:C(X)CHO with acyclic or cyclic
secondary amines R2NH lead to both the product of ipso-substitution of the
halogen atom and the products of fragmentation and condensation:
1,2-diaminoethenes R2NCH:CHNR2, carbonyl compds. R2COR1,
1,3-diamino-2-haloolefins R2R1(R2N)CC(X):CHNR2, and formamides R2NCHO.
The ratio of competitive reactions depends on the structure of the initial
aldehyde, the nature of amine, and exptl. conditions.
IT 176374-20-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of .alpha.-halo .alpha.,.beta.-unsatd. aldehydes with
secondary amines)
RN 176374-20-2 CAPLUS
CN Piperidine, 1,1'-(2-fluoro-3-methyl-1-propene-1,3-diyl)bis- (9CI) (CA
INDEX NAME)



L23 ANSWER 11 OF 15 USPATFULL

ACCESSION NUMBER: 2002:55187 USPATFULL

TITLE: Process for the preparation of chiral isofluoroenes

INVENTOR(S): Chiarello, John Francis, Newtown, PA, UNITED STATES

Buckwalter, Brian Lee, Yardley, PA, UNITED STATES

Barden, Timothy Claude, Holland, PA, UNITED STATES

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Ludwigshafen, GERMANY, FEDERAL
REPUBLIC OF (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002032351	A1	20020314
APPLICATION INFO.:	US 2001-921188	A1	20010802 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-222733P	20000803 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	Susan Shaw, Intellectual Property Department, BASF Corporation, 3000 Continental Drive - North, Mount Olive, NJ, 07828-1234	
NUMBER OF CLAIMS:	11	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1076	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB There is provided a process for the preparation of a chiral insecticidal and acaricidal compound of formula I. ##STR1##

Also provided are intermediate compounds useful in the process of the present invention.

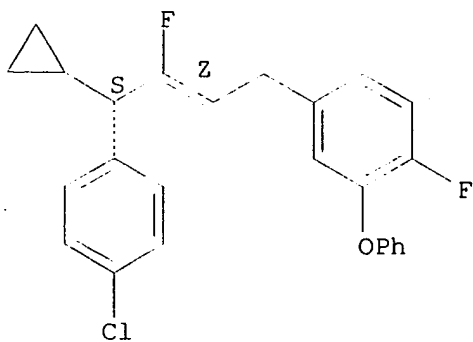
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 398453-72-0P, 4-[(2Z,4S)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene 398453-73-1P, 4-[(2E,4S)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene 398453-74-2P, 4-[(2E,4R)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene 398453-75-3P, 4-[(2Z,4R)-4-(4-Chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene (process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

RN 398453-72-0 USPATFULL

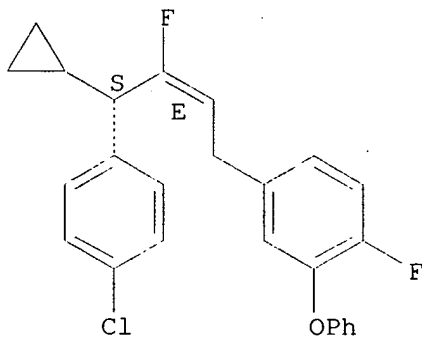
CN Benzene, 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



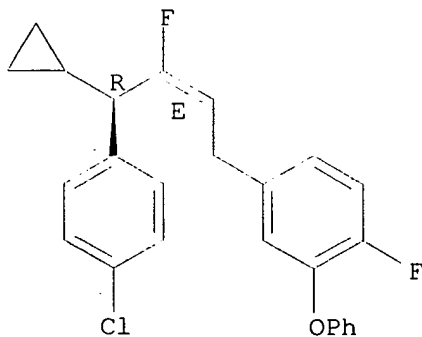
RN 398453-73-1 USPATFULL
CN Benzene, 4-[(2E,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



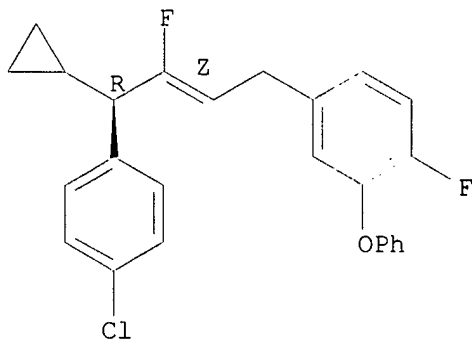
RN 398453-74-2 USPATFULL
CN Benzene, 4-[(2E,4R)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 398453-75-3 USPATFULL
CN Benzene, 4-[(2Z,4R)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L23 ANSWER 12 OF 15 USPATFULL

ACCESSION NUMBER: 2002:32732 USPATFULL

TITLE: Process for the preparation of 1,4-diaryl-2-fluoro-4-cyano-2-butenes and intermediates useful therefor

INVENTOR(S): Hu, Yulin, Plainsboro, NJ, UNITED STATES

Hunt, David Allen, Clifton Park, NY, UNITED STATES

PATENT ASSIGNEE(S): Intl Prop Dept, BASF Aktiengesellschaft, Ludwigshafen, GERMANY, FEDERAL REPUBLIC OF (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002019556	A1	20020214
	US 6444838	B2	20020903
APPLICATION INFO.:	US 2001-849298	A1	20010504 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-201826P	20000504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BASF Corporation, Intellectual Property Department, P.O. Box 400, Princeton, NJ, 08543-0400	
NUMBER OF CLAIMS:	15	
EXEMPLARY CLAIM:	1	
LINE COUNT:	471	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides a process for the preparation of
pesticidal 1,4-diaryl-2-fluoro-4-cyano-2 -butene compounds having the
structural formula I ##STR1##

and intermediates useful therefor

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 371759-00-1P

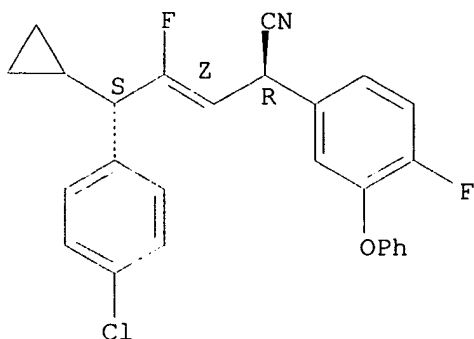
(prepn. of)

RN 371759-00-1 USPATFULL

CN Benzeneacetonitrile, .alpha.-[(1Z,3R)-3-(4-chlorophenyl)-3-cyclopropyl-2-
fluoro-1-propenyl]-4-fluoro-3-phenoxy-, (.alpha.S)-rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry.

Double bond geometry as shown.



L23 ANSWER 13 OF 15 USPATFULL

ACCESSION NUMBER: 2002:19447 USPATFULL

TITLE: 1,4-diaryl-2-fluoro-1-buten-3-ol compounds and their
use in the preparation of 1,4-diaryl-2-fluoro-1,3-
butadiene and 1,4-diaryl-2-fluoro-2-butene compounds

INVENTOR(S): Hu, Yulin, Plainsboro, NJ, United States
Hunt, David Allen, Clifton Park, NY, United States

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Ludwigshafen, GERMANY, FEDERAL
REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6342642	B1	20020129
	WO 2000029362		20000525
APPLICATION INFO.:	US 2001-856229		20010813 (9)
	WO 1999-US26434		19991109
			20010813 PCT 371 date
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Shippen, Michael L.		
LEGAL REPRESENTATIVE:	Maurer, Barbara V.		
NUMBER OF CLAIMS:	32		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)		
LINE COUNT:	851		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel 1,4-diaryl-2-fluoro-1-buten-3-ol
compounds of the structural formula I ##STR1##

a method for the preparation of those formula I compounds, and the use
of those formula I compounds in the preparation of 1,4-diaryl-2-fluoro-
1,3-butadiene compounds of formula II and 1,4-diaryl-2-fluoro-2-butene
compounds of formula III ##STR2##

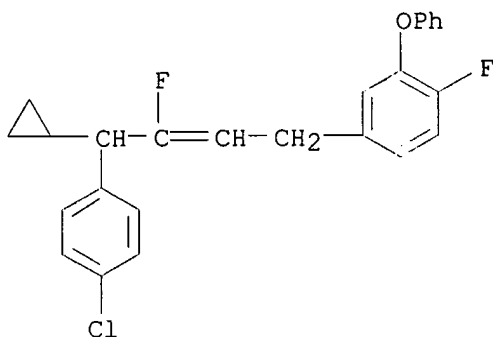
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 269398-40-5P 269398-41-6P

(prepn. of diarylfluorobutenol compds. and their use in the prepn. of
butadiene and butene derivs.)

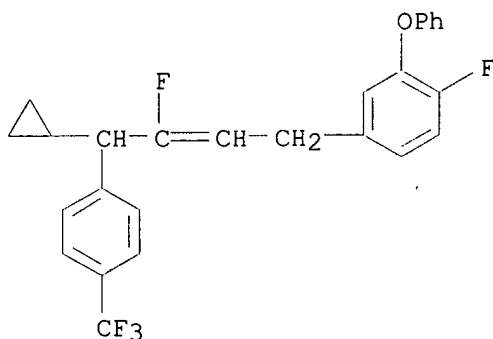
RN 269398-40-5 USPATFULL

CN Benzene, 4-[4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-
2-phenoxy- (9CI) (CA INDEX NAME)



RN 269398-41-6 USPATFULL

CN Benzene, 4-[4-cyclopropyl-3-fluoro-4-[4-(trifluoromethyl)phenyl]-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)



L23 ANSWER 14 OF 15 USPATFULL

ACCESSION NUMBER: 2001:158535 USPATFULL

TITLE: Processes for the preparation of 2-arylvinyl alkyl ether and 1,4-diaryl-2-fluoro-2-butene compounds

INVENTOR(S): Hu, Yulin, Plainsboro, NJ, United States
Hunt, David Allen, Newtown, PA, United States
Liu, Weiguo, Lawrenceville, NJ, United States

PATENT ASSIGNEE(S): American Cyanamid Co., Madison, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6291721	B1	20010918
APPLICATION INFO.:	US 1999-373262		19990812 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Keys, Rosalynd		
LEGAL REPRESENTATIVE:	Maurer, Barbara V.		
NUMBER OF CLAIMS:	22		
EXEMPLARY CLAIM:	1		
LINE COUNT:	894		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB An improved process for the preparation of 2-arylvinyl alkyl ether compounds of the structural formula I ##STR1##

In addition, the present invention provides an improved process for the preparation of 1,4-diaryl-2-fluoro-2-butene compounds of the structural formula V ##STR2##

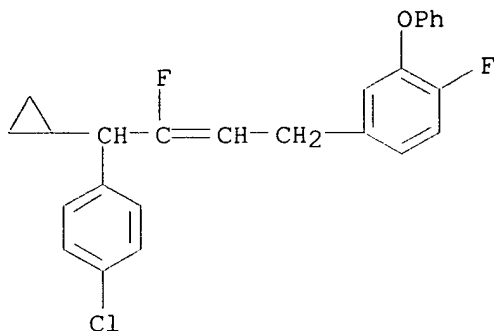
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 269398-40-5P

(prepn. of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes)

RN 269398-40-5 USPATFULL

CN Benzene, 4-[4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)



L23 ANSWER 15 OF 15 USPATFULL

ACCESSION NUMBER: 1998:157555 USPATFULL

TITLE: 1,4-diaryl-2-fluoro-2-butene insecticidal and acaricidal agents

INVENTOR(S): Barnes, Keith D., Newtown, PA, United States
Hu, Yulin, Plainsboro, NJ, United States

PATENT ASSIGNEE(S): American Cyanamid Company, Madison, NJ, United States
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5849958		19981215
APPLICATION INFO.:	US 1997-819623		19970317 (8)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Geist, Gary		
ASSISTANT EXAMINER:	Padmanabhan, Sreeni		
LEGAL REPRESENTATIVE:	Mazzarese, Joseph M.		
NUMBER OF CLAIMS:	6		
EXEMPLARY CLAIM:	1		
LINE COUNT:	934		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Pesticidal 1,4-diaryl-2-fluoro-2-butene compounds having the structural formula I ##STR1## and compositions and methods comprising those compounds for the control of insect and acarid pests.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 200401-86-1P 200401-93-0P 200401-94-1P

200401-95-2P 200401-96-3P 200401-97-4P

200401-98-5P 200401-99-6P 200402-00-2P

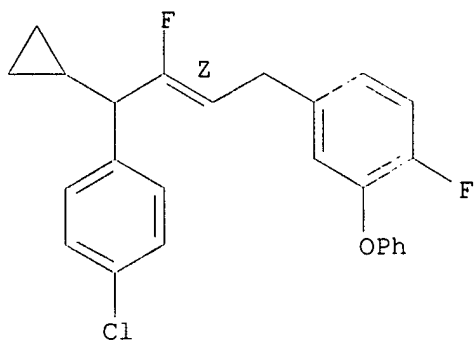
200402-01-3P 200402-02-4P 200402-03-5P

(prepn. of 1,4-diaryl-2-fluoro-2-butene insecticidal and acaricidal agents)

RN 200401-86-1 USPATFULL

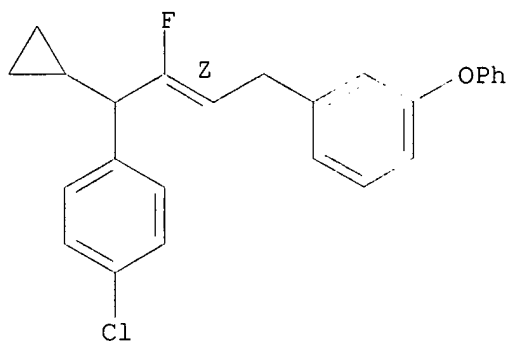
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



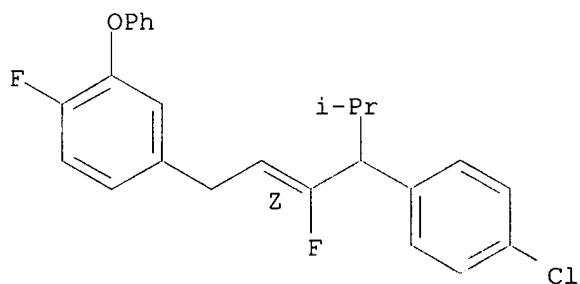
RN 200401-93-0 USPATFULL
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



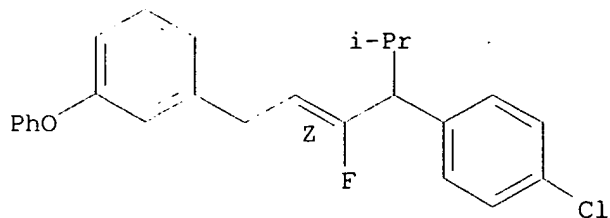
RN 200401-94-1 USPATFULL
CN Benzene, 4-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 200401-95-2 USPATFULL
CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

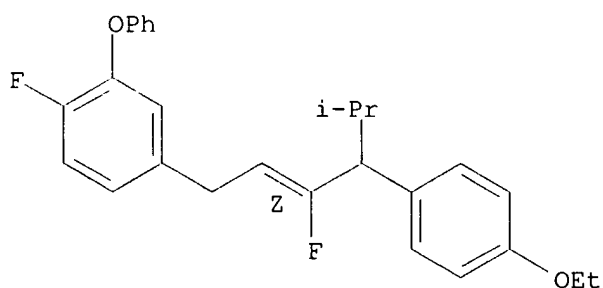
Double bond geometry as shown.



RN 200401-96-3 USPATFULL

CN Benzene, 4-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

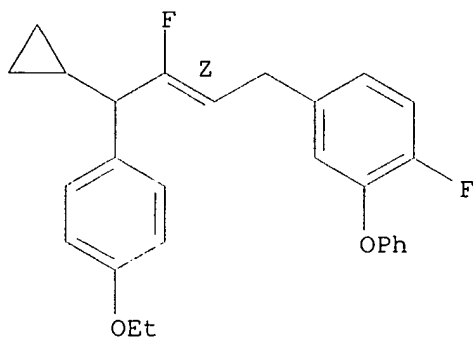
Double bond geometry as shown.



RN 200401-97-4 USPATFULL

CN Benzene, 4-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

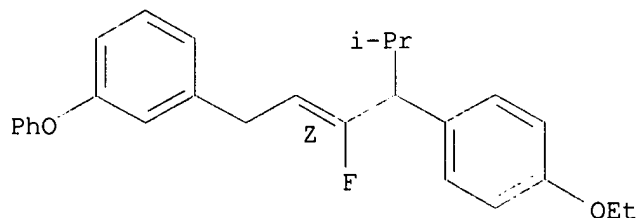
Double bond geometry as shown.



RN 200401-98-5 USPATFULL

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

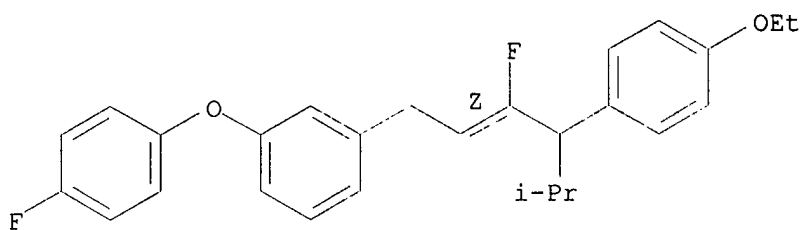
Double bond geometry as shown.



RN 200401-99-6 USPATFULL

CN Benzene, 1-[(2Z)-4-(4-ethoxyphenyl)-3-fluoro-5-methyl-2-hexenyl]-3-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

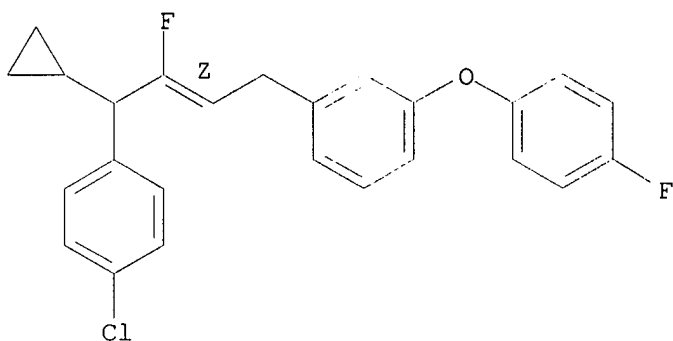
Double bond geometry as shown.



RN 200402-00-2 USPATFULL

CN Benzene, 1-[(2Z)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-3-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)

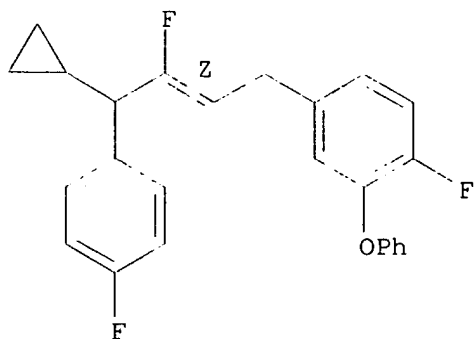
Double bond geometry as shown.



RN 200402-01-3 USPATFULL

CN Benzene, 4-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-1-fluoro-2-phenoxy- (9CI) (CA INDEX NAME)

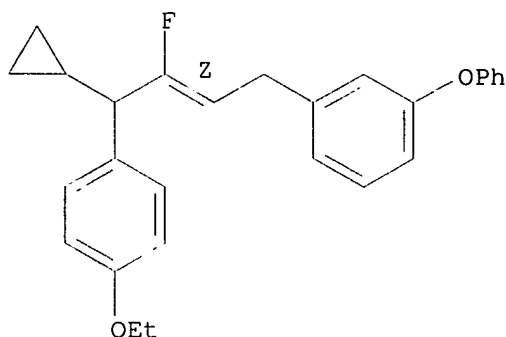
Double bond geometry as shown.



RN 200402-02-4 USPATFULL

CN Benzene, 1-[(2Z)-4-cyclopropyl-4-(4-ethoxyphenyl)-3-fluoro-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

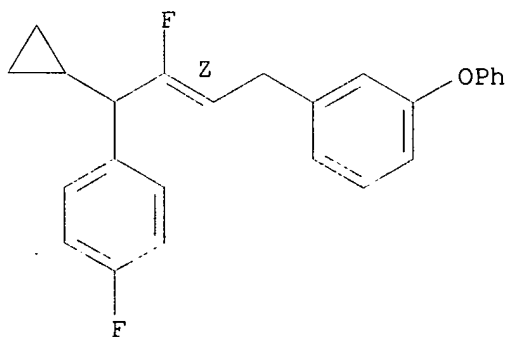
Double bond geometry as shown.



RN 200402-03-5 USPATFULL

CN Benzene, 1-[(2Z)-4-cyclopropyl-3-fluoro-4-(4-fluorophenyl)-2-butenyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



FILE 'CAOLD' ENTERED AT 11:50:31 ON 28 JAN 2003

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L22 0 SEA FILE=CAOLD ABB=ON L14

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FILE 'CASREACT' ENTERED AT 12:05:39 ON 28 JAN 2003
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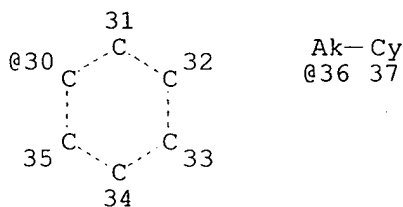
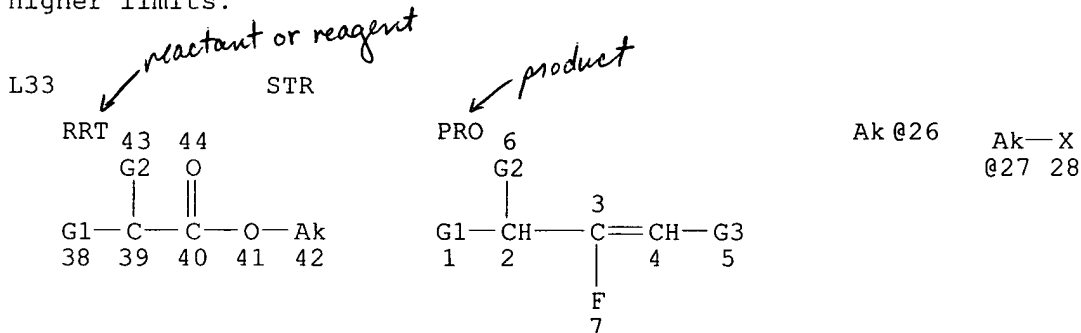
FILE CONTENT:1907 - 26 Jan 2003 VOL 138 ISS 4

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.



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VAR G2=26/27/CB
VAR G3=30/HY/36
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 26
CONNECT IS E1 RC AT 42
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L35 1 SEA FILE=CASREACT SSS FUL L33 (22 REACTIONS)

100.0% DONE 3154 VERIFIED 22 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.01

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L35 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 136:183615 CASREACT

TITLE: Process for the preparation of chiral insecticidal and acaricidal 1,4-diaryl-2-fluoro-2-butenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid methyl ester using esterase

INVENTOR(S): Chiarello, John Francis; Buckwalter, Brian Lee; Barden, Timothy Claude

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012155	A2	20020214	WO 2001-EP9012	20010803
WO 2002012155	A3	20021128		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2002032351	A1	20020314	US 2001-921188	20010802
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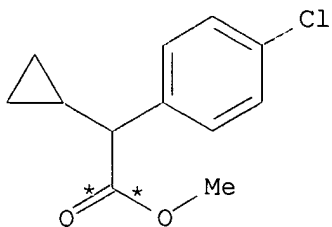
OTHER SOURCE(S): MARPAT 136:183615

AB There is provided a process for the prepn. of a chiral compd. of formula $\text{ArC}^*\text{H(R)CF:CHAr1}$ [I; Ar, Ar1 = (un)substituted aryl or a 5- or 6-membered heteroarom. ring; R is C1-4 alkyl, C1-4 haloalkyl, C3-6 cycloalkyl or C3-6 halocycloalkyl; Ar1, is aryl or a 5- or 6-membered heteroarom. ring; C* represents an asym. center] which is useful as an insecticidal and acaricidal agent and for protecting plants from damage caused by insect and acarid attack and infestation (no data). Also provided are intermediate compds. useful in the process of the present invention. This process comprises (a) treating a racemic ester of formula ArCH(R)CO2R4 (II; Ar, R = same as above; R4 = C1-4 alkyl) with an esterase to form a first mixt. of either R-acid of formula ArCH(R)CO2H (III) and S-ester of formula II or of S-acid of formula III and R-ester of formula II, (b) sepg. (R)- or (S)-acid III from said (S)- or (R)-ester II, (c) reducing the chiral acid (R)- or (S)-acid III or (S)- or (R)-ester II to obtain a chiral alc. of formula (R)- or (S)- $\text{ArC}^*\text{H(R)CH2OH}$, (d) transforming the chiral alc. into an ester (R)- or (S)- $\text{ArC}^*\text{H(R)CH2CO2R1}$, (e) fluorinating the latter ester to afford a fluoro-ester (R)- or (S)- $\text{ArC}^*\text{H(R)CHFCO2R1}$, and (f) reacting the latter fluoro-ester with an aldehyde Ar1CH2CHO (Ar1 = same as above) in a solvent in the presence of a base to afford a second mixt. of 4 chiral diastereomeric hydroxy-esters $\text{ArC}^*\text{H(R)CHF(CO2R1)CH(OH)CH2Ar1}$. It further comprises (g) optionally sepg. the second mixt. into a third mixt. each having two chiral diastereomers,

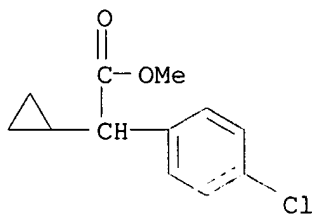
(h) treating the hydroxy-ester mixts. with an acylating agent R2COX1 (R2 = C1-4 alkyl; X1 = Cl, Br, R2CO2) to afford a fifth mixt. of 4 chiral diastereomeric acyloxy esters or a seventh mixt. of two chiral diastereomeric acyloxy esters $\text{ArC}^*\text{H(R)CHF(CO}_2\text{R}_1\text{)CH(O}_2\text{CR}_2\text{)CH}_2\text{Ar}_1$, (i) optionally sepg. the sixth or seventh mixt. not essentially pure chiral diastereomeric acyloxy ester, (j) hydrolyzing the pure acyloxy esters or mixts. of esters to afford a hydroxy acid $\text{ArC}^*\text{H(R)CHF(CO}_2\text{H)CH(OH)CH}_2\text{Ar}_1$, and (k) heating the hydroxy acid with a arylsulfonyl halide to afford I. Thus, Me (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate was treated with horse liver esterase in water (pH 7.5) to give 37.9% (2R)-(4-chlorophenyl)(cyclopropyl)ethanoic acid and 36.2% Me (2S)-(4-chlorophenyl)(cyclopropyl)ethanoate, each of which was reduced by $\text{BH}_3\cdot\text{THF/THF}$ at room temp. for 4 h and DIBAL/ CH_2Cl_2 warming from -78.degree. to room temp. and at room temp. for 1 h, resp., to give 84% (2R)-(4-chlorophenyl)(cyclopropyl)ethanol and 80% (2S)-(4-chlorophenyl)(cyclopropyl)ethanol, resp. Each of (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethanol was tosylated by tosyl chloride in the presence of Et3N in CH_2Cl_2 to (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethyl p-toluenesulfonate, resp., which underwent cyanation with NaCN in DMSO at 90.degree. for 3 h to give (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile, resp. Alkali hydrolysis of (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile in a mixt. of 10% aq. NaOH and methanol under reflux for 18 h followed by acidification with concd. HCl gave (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoic acid, resp., which was esterified with MeOH in the presence of HCl at room temp. for 18 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate, resp. Lithiation of the each ester with lithium diisopropylamide (LDA) in THF at -78.degree. to 0.degree. followed by fluorination with $(\text{PhSO}_2)_2\text{NF}$ at -78.degree. to room temp. and room temp. for 2 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate, resp. Lithiation of Me (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate with LDA in THF at -78.degree. for 15 min followed by addn. reaction with 4-fluoro-3-phenoxyphenylacetaldehyde at -78.degree. for 2 h gave, after silica gel chromatog., an oil (A) contg. (2R,3R) and (2R,3S) or (2S,3R)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate and an oil contg. (2S,3S) and (2S,3R) or (2R,3S)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate (steps f and g). Acetylation of the oil A with Ac_2O in the presence of DAMP in CH_2Cl_2 at room temp. for 2 h gave Me (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate and Me (2R,3S or 2S,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate (step h and i). Alkali hydrolysis of the latter diastereomer in a mixt. of 10% aq. NaOH, MeOH, and THF under reflux for 1 h gave (2S,3R or 2R,3S)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid (step j) which was heated with tosyl chloride in collidine at 170.degree. for 2 h to give 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene as a colorless oil (step k).

RX(349) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14),
RX(30), RX(25), RX(29)

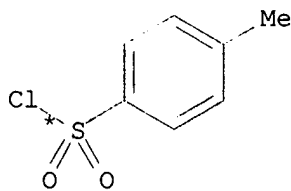
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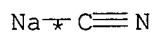
4 G



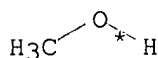
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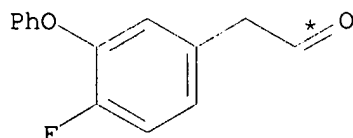
J



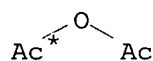
O



4 V

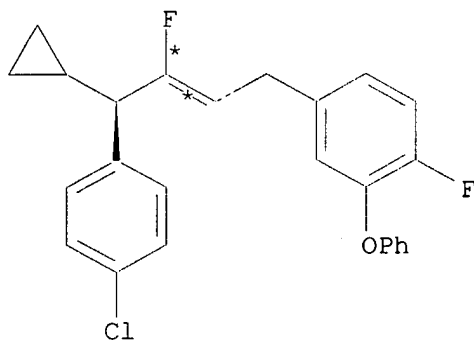


4 AD



2 BG

10
STEPS
→



BF

- RX(3) RCT G **119544-56-8**
 PRO A 398453-51-5, E 398453-52-6
 CAT 9016-18-6 Carbonic esterase
 SOL 7732-18-5 Water
 NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(1) RCT A 398453-51-5
 RGT C 14044-65-6 BH3-THF
 PRO B 119544-59-1
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h
- RX(4) RCT B 119544-59-1, J 98-59-9
 RGT L 121-44-8 Et3N
 PRO K 398453-53-7
 SOL 75-09-2 CH2Cl2
 NTE tosylation at room temp. for 3 days
- RX(6) RCT K 398453-53-7, O 143-33-9
 PRO P 398453-55-9

SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(30) RCT AE 398464-67-0, AG 398464-70-5, BG 108-24-7
PRO BH 398453-68-4, BC 398453-80-0
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(25) RCT BC 398453-80-0

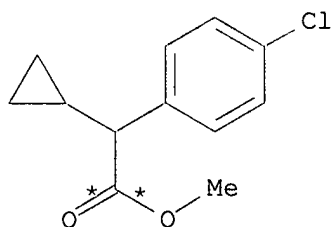
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO BD 398453-84-4
NTE sapon. under reflux for 1 h; acidification with concd. HCl

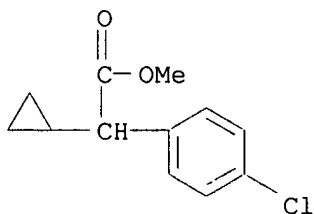
RX(29) RCT BD 398453-84-4
RGT J 98-59-9 TsCl
PRO BF 398453-75-3
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(350) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14),
RX(31), RX(25), RX(29)

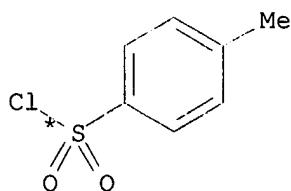
RX(350) 5 G + J + O + 4 V + 4 AD + 2 BG ==> BF



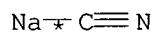
4 G



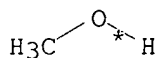
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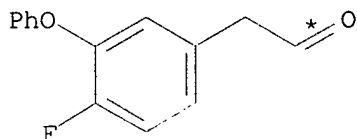
J



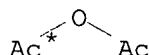
O



4 V

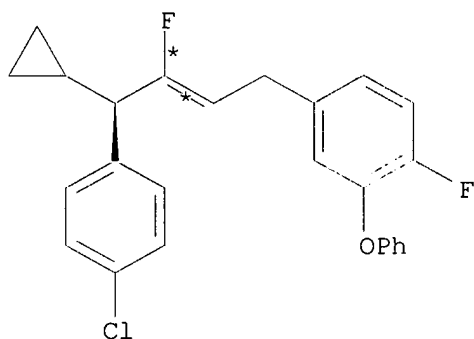


4 AD



2 BG

10
STEPS
→



BF

- RX(3) RCT G **119544-56-8**
 PRO A 398453-51-5, E 398453-52-6
 CAT 9016-18-6 Carbonic esterase
 SOL 7732-18-5 Water
 NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(1) RCT A 398453-51-5
 RGT C 14044-65-6 BH3-THF
 PRO B 119544-59-1
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h
- RX(4) RCT B 119544-59-1, J 98-59-9
 RGT L 121-44-8 Et3N
 PRO K 398453-53-7

SOL 75-09-2 CH₂Cl₂
NTE tosylation at room temp. for 3 days

RX(6) RCT K 398453-53-7, O 143-33-9
PRO P 398453-55-9
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO₂)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(31) RCT AF 398464-69-2, AG 398464-70-5, BG 108-24-7
PRO AR 398453-67-3, BC 398453-80-0
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
NTE acetylation at room temp. for 2 h

RX(25) RCT BC 398453-80-0

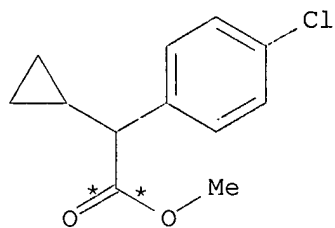
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO BD 398453-84-4
NTE sapon. under reflux for 1 h; acidification with concd. HCl

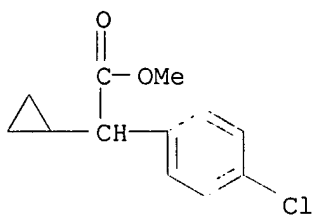
RX(29) RCT BD 398453-84-4
RGT J 98-59-9 TsCl
PRO BF 398453-75-3
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(351) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14),
RX(31), RX(18), RX(21)

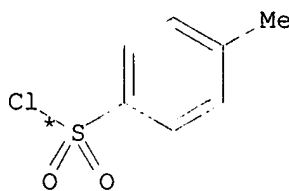
RX(351) 5 G + J + O + 4 V + 4 AD + 2 BG ==> AV



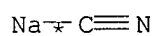
4 G



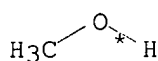
G



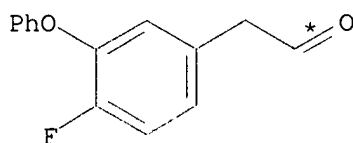
J



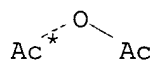
O



4 V

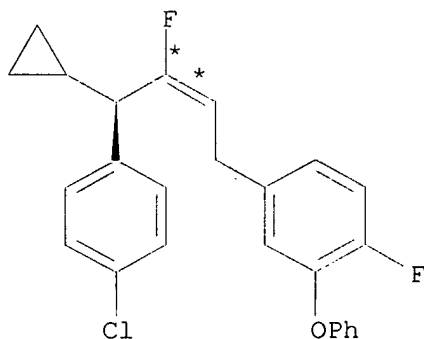


4 AD



2 BG

10
STEPS
→



AV

RX(3) RCT G **119544-56-8**
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(1) RCT A 398453-51-5
RGT C 14044-65-6 BH3-THF
PRO B 119544-59-1
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(4) RCT B 119544-59-1, J 98-59-9
RGT L 121-44-8 Et3N
PRO K 398453-53-7
SOL 75-09-2 CH2Cl2

NTE tosylation at room temp. for 3 days

RX(6) RCT K 398453-53-7, O 143-33-9
PRO P 398453-55-9
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(31) RCT AF 398464-69-2, AG 398464-70-5, BG 108-24-7
PRO AR 398453-67-3, BC 398453-80-0
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(18) RCT AR 398453-67-3

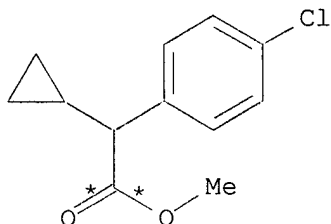
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AS 398453-71-9
NTE sapon. under reflux for 1 h; acidification with concd. HCl

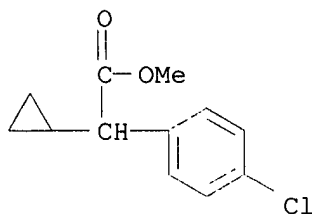
RX(21) RCT AS 398453-71-9
RGT J 98-59-9 TsCl
PRO AV 398453-74-2
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(352) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14),
RX(33), RX(18), RX(21)

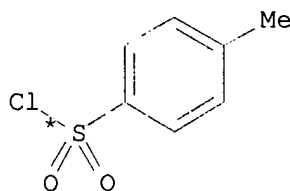
RX(352) 5 G + J + O + 4 V + 4 AD + 2 BG ==> AV



4 G



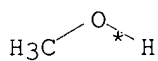
G



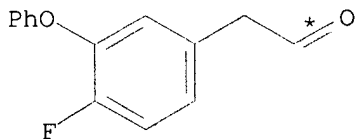
J

Na-C≡N

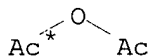
O



4 V

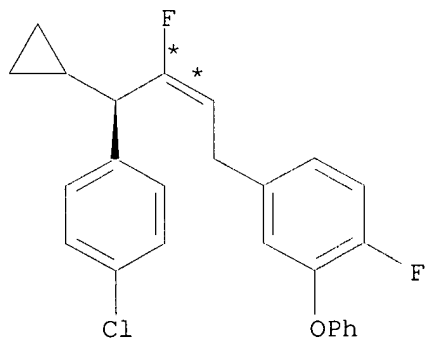


4 AD



2 BG

10
STEPS
→



AV

RX(3) RCT G 119544-56-8
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(1) RCT A 398453-51-5
RGT C 14044-65-6 BH3-THF
PRO B 119544-59-1
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(4) RCT B 119544-59-1, J 98-59-9
RGT L 121-44-8 Et3N
PRO K 398453-53-7
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(6) RCT K 398453-53-7, O 143-33-9
PRO P 398453-55-9
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(33) RCT AH 398464-71-6, AF 398464-69-2, BG 108-24-7
PRO AR 398453-67-3, BA 398453-79-7
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(18) RCT AR 398453-67-3

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AS 398453-71-9
NTE sapon. under reflux for 1 h; acidification with concd. HCl

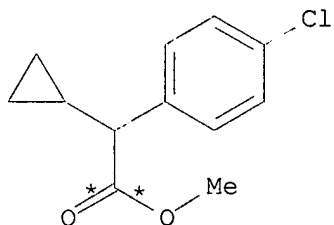
RX(21) RCT AS 398453-71-9
RGT J 98-59-9 TsCl
PRO AV 398453-74-2

SOL 29611-84-5 Collidine

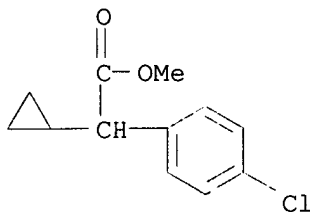
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(353) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14), RX(32), RX(24), RX(28)

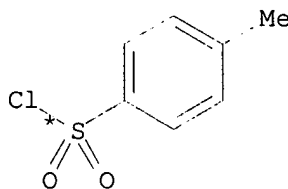
RX(353) 5 G + J + O + 4 V + 4 AD + 2 BG ==> BF



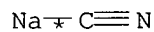
4 G



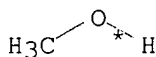
G



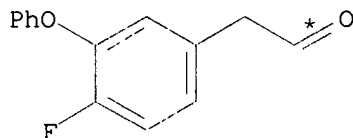
J



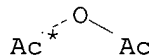
O



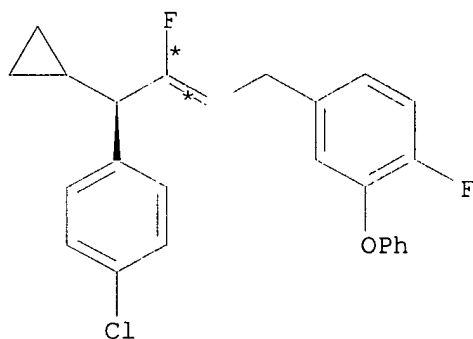
4 V



4 AD



2 BG

10
STEPS
→

BF

RX(3)

RCT G 119544-56-8

PRO A 398453-51-5, E 398453-52-6

CAT 9016-18-6 Carbonic esterase

SOL 7732-18-5 Water

NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(1)

RCT A 398453-51-5

RGT C 14044-65-6 BH3-THF

PRO B 119544-59-1

SOL 109-99-9 THF

NTE redn. at room temp. for 4 h

RX(4) RCT B 119544-59-1, J 98-59-9
RGT L 121-44-8 Et3N
PRO K 398453-53-7
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(6) RCT K 398453-53-7, O 143-33-9
PRO P 398453-55-9
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(32) RCT AH 398464-71-6, AE 398464-67-0, BG 108-24-7
PRO BH 398453-68-4, BA 398453-79-7
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(24) RCT BA 398453-79-7

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

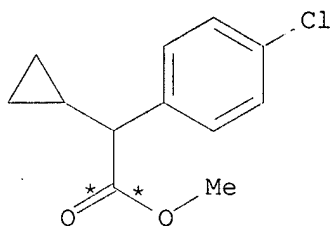
STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO BB 398453-76-4
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(28) RCT BB 398453-76-4
RGT J 98-59-9 TsCl
PRO BF 398453-75-3
SOL 29611-84-5 Collidine

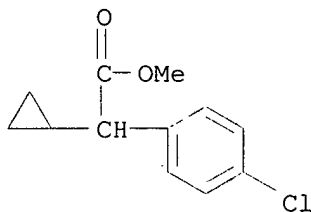
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(354) OF 398 COMPOSED OF RX(3), RX(1), RX(4), RX(6), RX(9), RX(12), RX(14), RX(33), RX(24), RX(28)

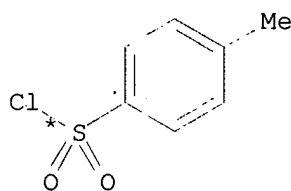
RX(354) 5 G + J + O + 4 V + 4 AD + 2 BG ==> BF



4 G



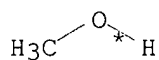
G



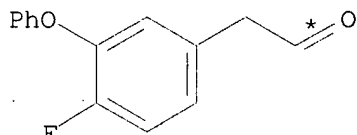
J

Na-C≡N

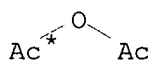
O



4 V

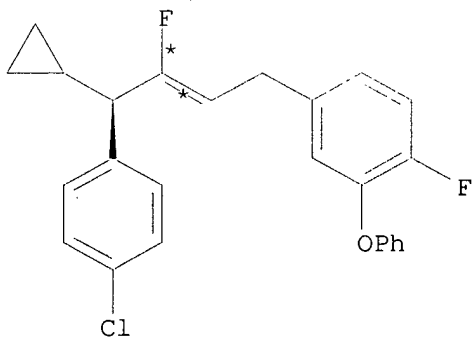


4 AD



2 BG

10
STEPS
→



BF

RX(3) RCT G 119544-56-8
 PRO A 398453-51-5, E 398453-52-6
 CAT 9016-18-6 Carbonic esterase
 SOL 7732-18-5 Water
 NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(1) RCT A 398453-51-5

RGT C 14044-65-6 BH3-THF
PRO B 119544-59-1
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(4) RCT B 119544-59-1, J 98-59-9
RGT L 121-44-8 Et3N
PRO K 398453-53-7
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(6) RCT K 398453-53-7, O 143-33-9
PRO P 398453-55-9
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(9) RCT P 398453-55-9, V 67-56-1
PRO W 398453-59-3
CAT 7647-01-0 HCl
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(12) RCT W 398453-59-3

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO Z 398453-61-7
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(14) RCT Z 398453-61-7

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AE 398464-67-0, AF 398464-69-2, AG 398464-70-5, AH 398464-71-6
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h

RX(33) RCT AH 398464-71-6, AF 398464-69-2, BG 108-24-7
PRO AR 398453-67-3, BA 398453-79-7
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(24) RCT BA 398453-79-7

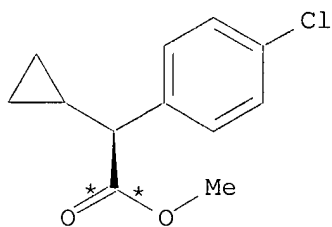
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO BB 398453-76-4
NTE sapon. under reflux for 1 h; acidification with concd. HCl

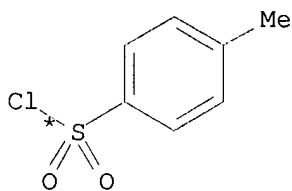
RX(28) RCT BB 398453-76-4
 RGT J 98-59-9 TsCl
 PRO BF 398453-75-3
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(383) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
 RX(34), RX(17), RX(19)

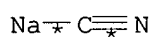
RX(383) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
 AT



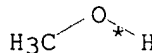
4 E



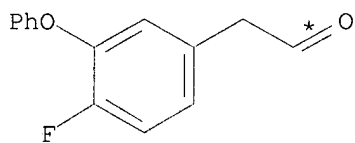
4 J



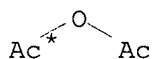
4 O



4 V

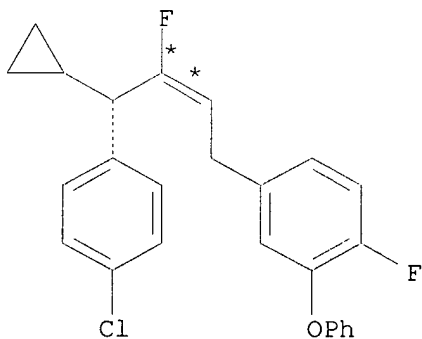


4 AD



2 BG

10
 STEPS
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AT

RX(2) RCT E 398453-52-6
 RGT C 14044-65-6 BH3-THF
 PRO F 119544-60-4
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
 RGT L 121-44-8 Et3N

PRO N 398453-54-8
SOL 75-09-2 CH₂Cl₂
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO₂)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(34) RCT AI 398464-73-8, AL 398464-76-1, BG 108-24-7
PRO AP 398453-64-0, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
NTE acetylation at room temp. for 2 h

RX(17) RCT AP 398453-64-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

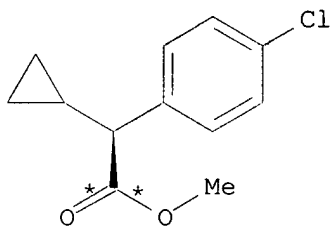
RGT U 7647-01-0 HCl
 SOL 141-78-6 AcOEt
 PRO AQ 398453-69-5
 NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(19) RCT AQ 398453-69-5
 RGT J 98-59-9 TsCl
 PRO AT 398453-73-1
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

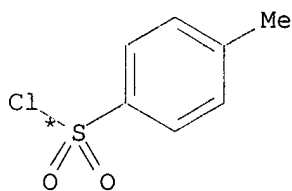
RX(384) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
 RX(35), RX(17), RX(19)

RX(384) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

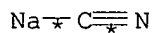
AT



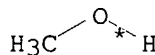
4 E



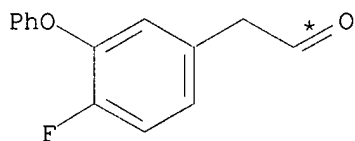
4 J



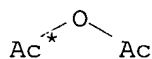
4 O



4 V

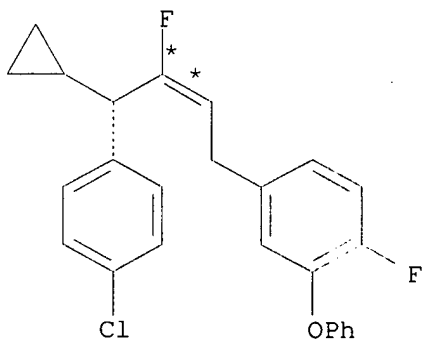


4 AD



2 BG

10
STEPS
→



AT

RX(2) RCT E 398453-52-6
 RGT C 14044-65-6 BH3-THF

PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(35) RCT AI 398464-73-8, AK 398464-75-0, BG 108-24-7
PRO AP 398453-64-0, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(17) RCT AP 398453-64-0

STAGE(1)

RGT T 1310-73-2 NaOH

SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

RGT U 7647-01-0 HCl

SOL 141-78-6 AcOEt

PRO AQ 398453-69-5

NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(19) RCT AQ 398453-69-5

RGT J 98-59-9 TsCl

PRO AT 398453-73-1

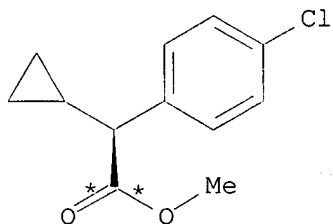
SOL 29611-84-5 Collidine

NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

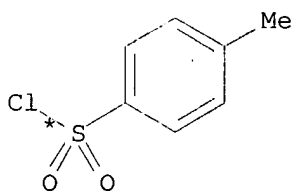
RX(385) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
RX(34), RX(22), RX(26)

RX(385) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

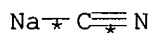
BE



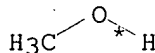
4 E



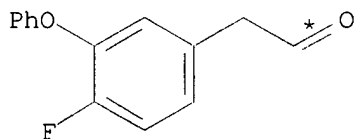
4 J



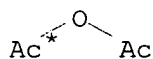
4 O



4 V

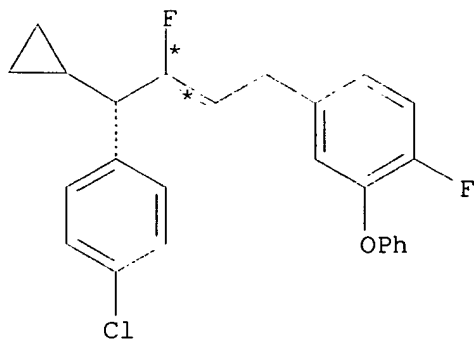


4 AD



2 BG

10
STEPS
→



BE
YIELD 69%

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)

RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8

NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at
-78.degree. for 2 h; 50% overall yield

RX(34) RCT AI 398464-73-8, AL 398464-76-1, BG 108-24-7
PRO AP 398453-64-0, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
NTE acetylation at room temp. for 2 h

RX(22) RCT AW 398453-77-5

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

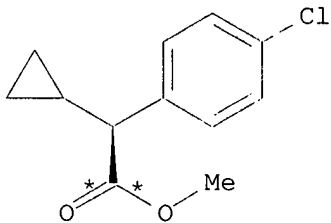
STAGE(2)

RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AX 398453-81-1
NTE sapon. under reflux for 1 h; acidification with concd. HCl

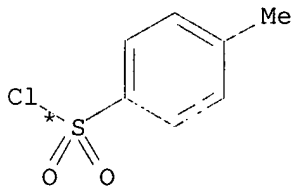
RX(26) RCT AX 398453-81-1
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for
2 h

RX(386) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
RX(36), RX(22), RX(26)

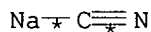
RX(386) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
BE



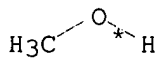
4 E



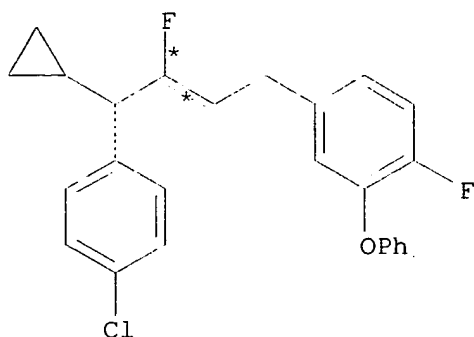
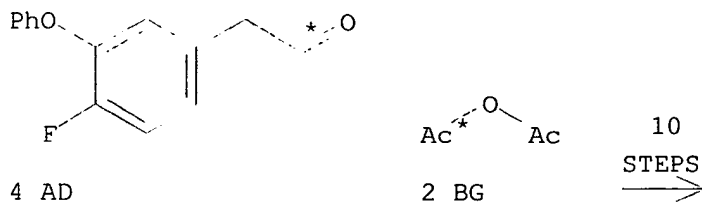
4 J



4 O



4 V



BE
YIELD 69%

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)

RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl

NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at
-78.degree. for 2 h; 50% overall yield

RX(36) RCT AJ 398464-74-9, AL 398464-76-1, BG 108-24-7
PRO AM 398453-63-9, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h in 79% overall yield

RX(22) RCT AW 398453-77-5

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

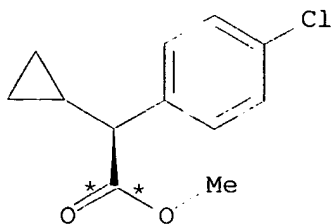
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AX 398453-81-1
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(26) RCT AX 398453-81-1
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for
2 h

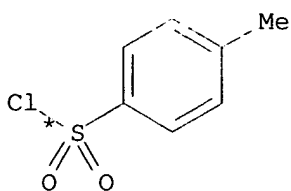
RX(387) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
RX(35), RX(23), RX(27)

RX(387) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

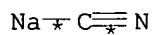
BE



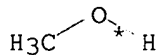
4 E



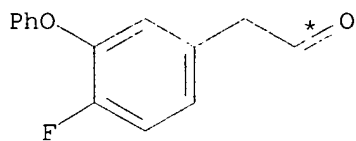
4 J



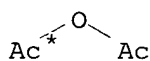
4 O



4 V

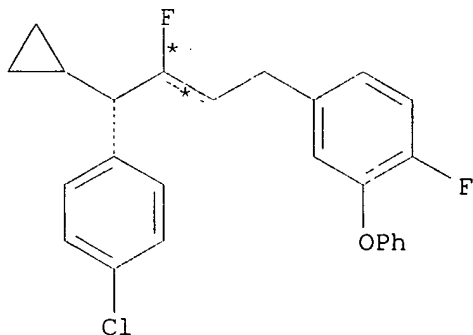


4 AD



2 BG

10
STEPS
→



BE
YIELD 69%

- RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h
- RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days
- RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h
- RX(10) RCT R 398453-56-0

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)

RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO₂)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)₂
SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(35) RCT AI 398464-73-8, AK 398464-75-0, BG 108-24-7
PRO AP 398453-64-0, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
NTE acetylation at room temp. for 2 h

RX(23) RCT AY 398453-78-6

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

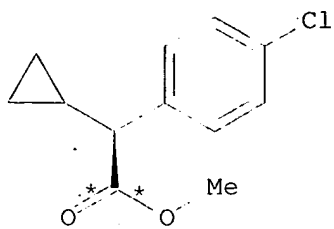
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AZ 398453-82-2
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(27) RCT AZ 398453-82-2
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for

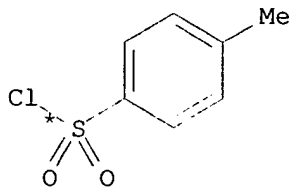
2 h

RX(388) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
RX(37), RX(23), RX(27)

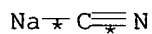
RX(388) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
BE



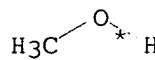
4 E



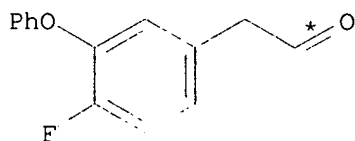
4 J



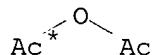
4 O



4 V

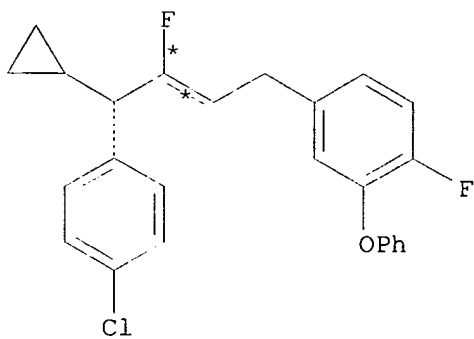


4 AD



2 BG

10
STEPS
→



BE
YIELD 69%

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min; fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(37) RCT AK 398464-75-0, AJ 398464-74-9, BG 108-24-7
PRO AM 398453-63-9, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(23) RCT AY 398453-78-6

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

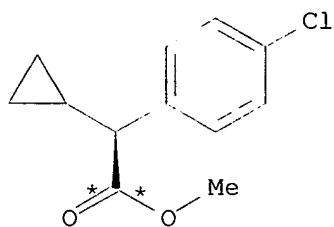
STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AZ 398453-82-2

NTE sapon. under reflux for 1 h; acidification with concd. HCl

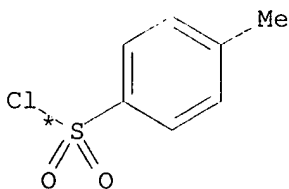
RX(27) RCT AZ 398453-82-2
 RGT J 98-59-9 TsCl
 PRO BE 398453-72-0
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(389) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
 RX(36), RX(16), RX(20)

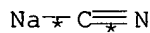
RX(389) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
 AT



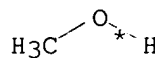
4 E



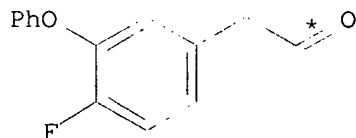
4 J



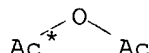
4 O



4 V

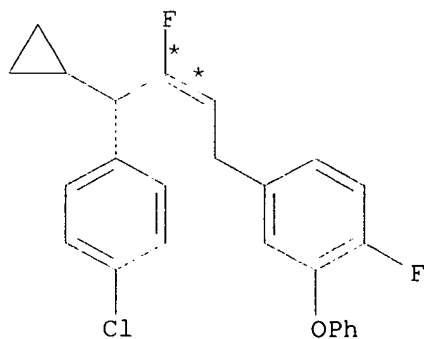


4 AD



2 BG

10
 STEPS
 —————>



AT

RX(2) RCT E 398453-52-6
 RGT C 14044-65-6 BH3-THF
 PRO F 119544-60-4
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(36) RCT AJ 398464-74-9, AL 398464-76-1, BG 108-24-7
PRO AM 398453-63-9, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h in 79% overall yield

RX(16) RCT AM 398453-63-9

STAGE(1)
RGT T 1310-73-2 NaOH

SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

RGT U 7647-01-0 HCl

SOL 141-78-6 AcOEt

PRO AN 398453-70-8

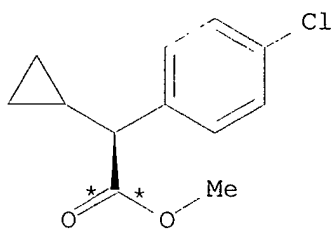
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(20) RCT AN 398453-70-8
 RGT J 98-59-9 TsCl
 PRO AT **398453-73-1**
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

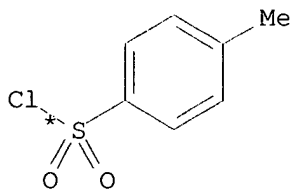
RX(390) OF 398 COMPOSED OF RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15),
 RX(37), RX(16), RX(20)

RX(390) 4 E + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

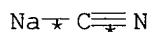
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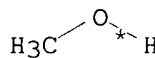
4 E



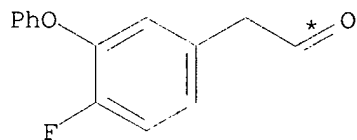
4 J



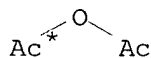
4 O



4 V

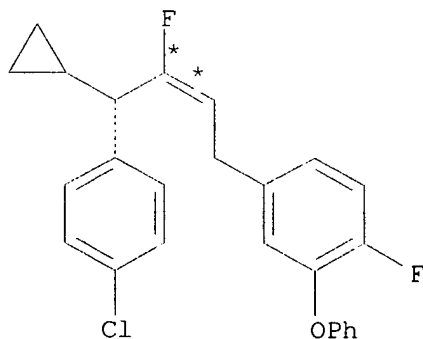


4 AD



2 BG

10
 STEPS
 —>



AT

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min; fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(37) RCT AK 398464-75-0, AJ 398464-74-9, BG 108-24-7
PRO AM 398453-63-9, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

NTE acetylation at room temp. for 2 h

RX(16) RCT AM 398453-63-9

STAGE(1)

RGT T 1310-73-2 NaOH

SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

RGT U 7647-01-0 HCl

SOL 141-78-6 AcOEt

PRO AN 398453-70-8

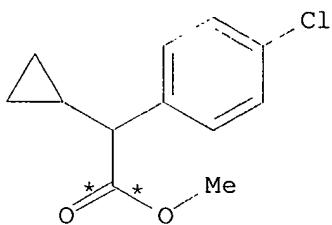
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(20) RCT AN 398453-70-8
 RGT J 98-59-9 TsCl
 PRO AT **398453-73-1**
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

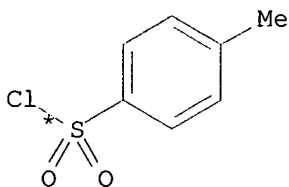
RX(391) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
 RX(15), RX(34), RX(17), RX(19)

RX(391) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

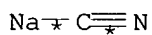
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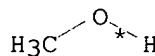
5 G



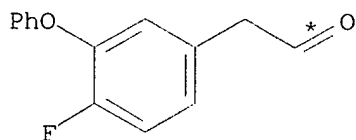
4 J



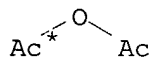
4 O



4 V

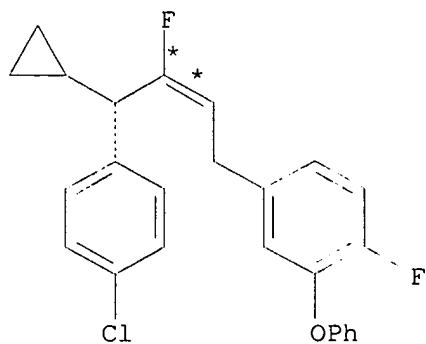


4 AD



2 BG

11
 STEPS
 →



AT

- RX(3) RCT G 119544-56-8
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h
- RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days
- RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h
- RX(10) RCT R 398453-56-0
- STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
- STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.
- RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h
- RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)₂
 SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO₂)NF
 PRO AC 398453-62-8
 NTE deprotonation at -78.degree. to 0.degree. over 5 min;
 fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)₂
 SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
 PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
 NTE deprotonation at -78.degree. for 15 min; addn. reaction at
 -78.degree. for 2 h; 50% overall yield

RX(34) RCT AI 398464-73-8, AL 398464-76-1, BG 108-24-7
 PRO AP 398453-64-0, AW 398453-77-5
 CAT 1122-58-3 4-DMAP
 SOL 75-09-2 CH₂Cl₂
 NTE acetylation at room temp. for 2 h

RX(17) RCT AP 398453-64-0

STAGE(1)

RGT T 1310-73-2 NaOH
 SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

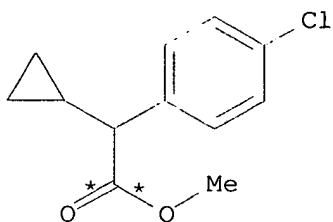
RGT U 7647-01-0 HCl
 SOL 141-78-6 AcOEt
 PRO AQ 398453-69-5
 NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(19) RCT AQ 398453-69-5
 RGT J 98-59-9 TsCl
 PRO AT **398453-73-1**
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for
 2 h

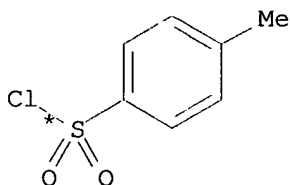
RX(392) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
 RX(15), RX(35), RX(17), RX(19)

RX(392) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

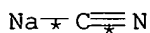
AT



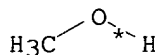
5 G



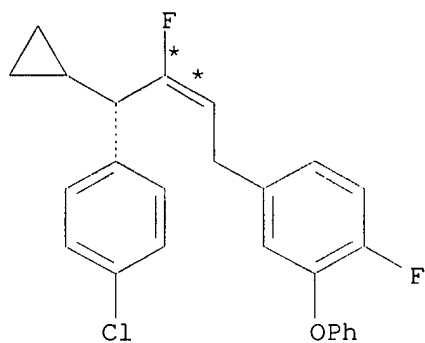
4 J



4 O



4 V



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RX(3)      RCT  G 119544-56-8
           PRO  A 398453-51-5, E 398453-52-6
           CAT  9016-18-6 Carbonic esterase
           SOL  7732-18-5 Water
           NTE  biotransformation; enzymic stereoselective hydrolysis at room
                temp. and pH 7.1-8.0

RX(2)      RCT  E 398453-52-6
           RGT  C 14044-65-6 BH3-THF
           PRO  F 119544-60-4
           SOL  109-99-9 THF
           NTE  redn. at room temp. for 4 h

RX(5)      RCT  F 119544-60-4, J 98-59-9
           RGT  L 121-44-8 Et3N
           PRO  N 398453-54-8
           SOL  75-09-2 CH2Cl2
           NTE  tosylation at room temp. for 3 days

RX(7)      RCT  N 398453-54-8, O 143-33-9
           PRO  R 398453-56-0
           SOL  67-68-5 DMSO
           NTE  cyanation at 90.degree. for 3 h

RX(10)     RCT  R 398453-56-0

           STAGE(1)
             RGT  T 1310-73-2 NaOH
             SOL  7732-18-5 Water, 67-56-1 MeOH

           STAGE(2)
             RGT  U 7647-01-0 HCl

```

SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(35) RCT AI 398464-73-8, AK 398464-75-0, BG 108-24-7
PRO AP 398453-64-0, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(17) RCT AP 398453-64-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

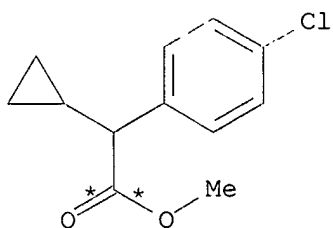
STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AQ 398453-69-5
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(19) RCT AQ 398453-69-5
RGT J 98-59-9 TsCl
PRO AT 398453-73-1
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

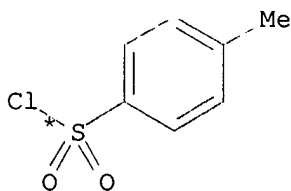
RX(393) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
RX(15), RX(34), RX(22), RX(26)

RX(393) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

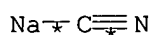
BE



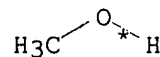
5 G



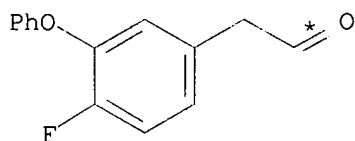
4 J



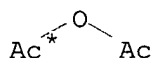
4 O



4 V

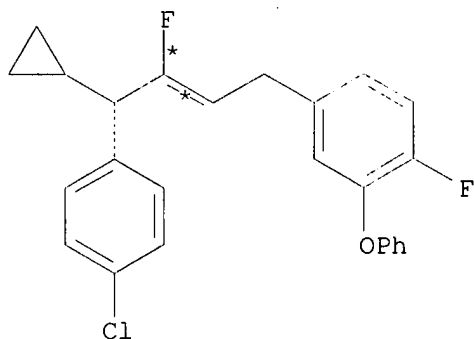


4 AD



2 BG

11
STEPS
→



BE
YIELD 69%

- RX(3) RCT G 119544-56-8
 PRO A 398453-51-5, E 398453-52-6
 CAT 9016-18-6 Carbonic esterase
 SOL 7732-18-5 Water
 NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(2) RCT E 398453-52-6
 RGT C 14044-65-6 BH3-THF
 PRO F 119544-60-4
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h
- RX(5) RCT F 119544-60-4, J 98-59-9
 RGT L 121-44-8 Et3N
 PRO N 398453-54-8
 SOL 75-09-2 CH2Cl2
 NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6
STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF
STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8
STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF
STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(34) RCT AI 398464-73-8, AL 398464-76-1, BG 108-24-7
PRO AP 398453-64-0, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(22) RCT AW 398453-77-5
STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water
STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt

PRO AX 398453-81-1

NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(26) RCT AX 398453-81-1

RGT J 98-59-9 TsCl

PRO BE **398453-72-0**

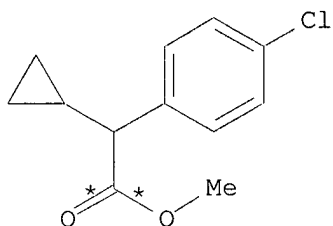
SOL 29611-84-5 Collidine

NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

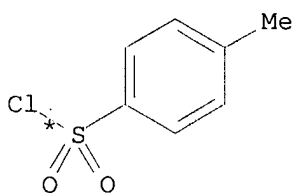
RX(394) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
RX(15), RX(36), RX(22), RX(26)

RX(394) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

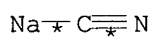
BE



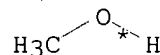
5 G



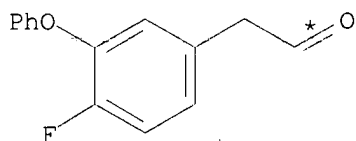
4 J



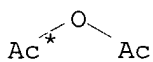
4 O



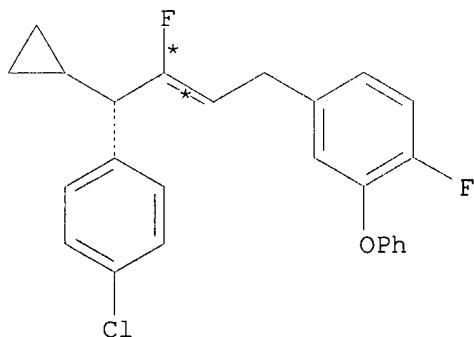
4 V



4 AD



2 BG

11
STEPS
→BE
YIELD 69%RX(3) RCT G **119544-56-8**

PRO A 398453-51-5, E 398453-52-6

CAT 9016-18-6 Carbonic esterase

SOL 7732-18-5 Water

NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min; fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(36) RCT AJ 398464-74-9, AL 398464-76-1, BG 108-24-7

PRO AM 398453-63-9, AW 398453-77-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
NTE acetylation at room temp. for 2 h in 79% overall yield

RX(22) RCT AW 398453-77-5

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

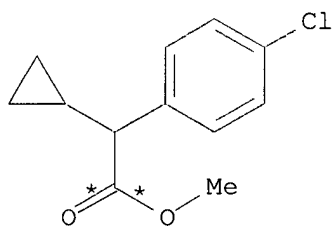
STAGE(2)

RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AX 398453-81-1
NTE sapon. under reflux for 1 h; acidification with concd. HCl

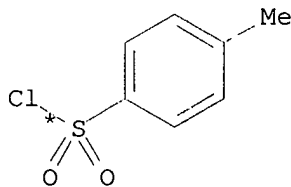
RX(26) RCT AX 398453-81-1
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

RX(395) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
RX(15), RX(35), RX(23), RX(27)

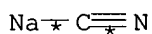
RX(395) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
BE



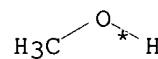
5 G



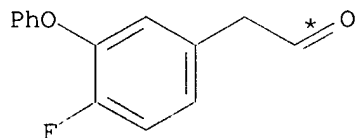
4 J



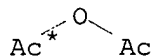
4 O



4 V

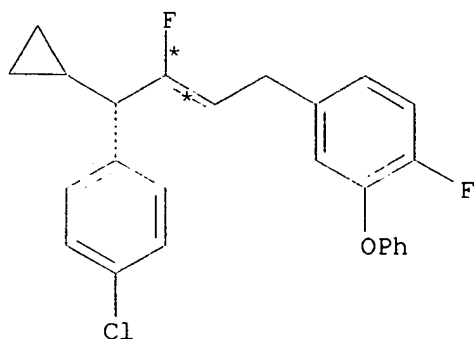


4 AD



2 BG

11
STEPS
=>



BE
YIELD 69%

RX(3) RCT G 119544-56-8
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at
-78.degree. for 2 h; 50% overall yield

RX(35) RCT AI 398464-73-8, AK 398464-75-0, BG 108-24-7
PRO AP 398453-64-0, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(23) RCT AY 398453-78-6

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

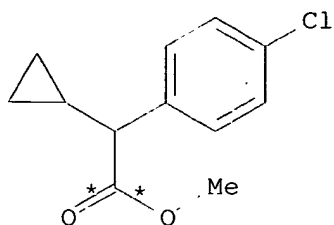
STAGE(2)

RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AZ 398453-82-2
NTE sapon. under reflux for 1 h; acidification with concd. HCl

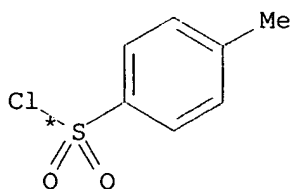
RX(27) RCT AZ 398453-82-2
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for
2 h

RX(396) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
RX(15), RX(37), RX(23), RX(27)

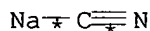
RX(396) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>
BE



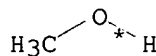
5 G



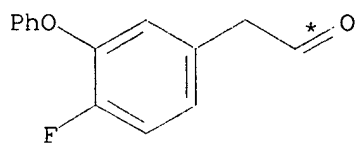
4 J



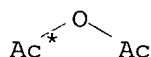
4 O



4 V

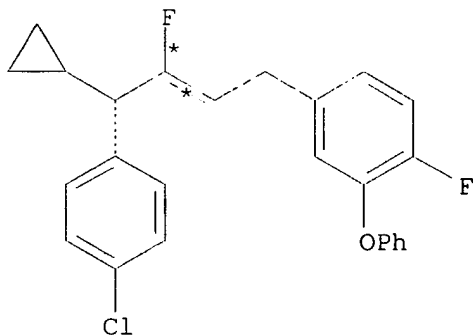


4 AD



2 BG

11
STEPS
→



BE
YIELD 69%

- RX(3) RCT G 119544-56-8
 PRO A 398453-51-5, E 398453-52-6
 CAT 9016-18-6 Carbonic esterase
 SOL 7732-18-5 Water
 NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(2) RCT E 398453-52-6
 RGT C 14044-65-6 BH3-THF
 PRO F 119544-60-4
 SOL 109-99-9 THF
 NTE redn. at room temp. for 4 h
- RX(5) RCT F 119544-60-4, J 98-59-9
 RGT L 121-44-8 Et3N
 PRO N 398453-54-8
 SOL 75-09-2 CH2Cl2
 NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min; fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(37) RCT AK 398464-75-0, AJ 398464-74-9, BG 108-24-7
PRO AM 398453-63-9, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(23) RCT AY 398453-78-6

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)
RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AZ 398453-82-2

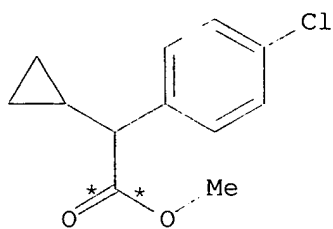
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(27) RCT AZ 398453-82-2
RGT J 98-59-9 TsCl
PRO BE 398453-72-0
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

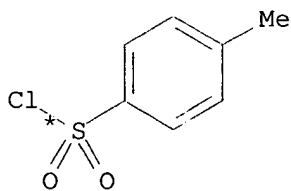
RX(397) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13), RX(15), RX(36), RX(16), RX(20)

RX(397) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

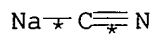
AT



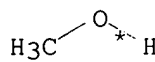
5 G



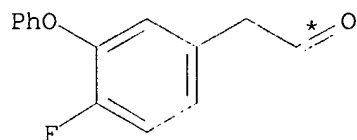
4 J



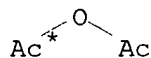
4 O



4 V

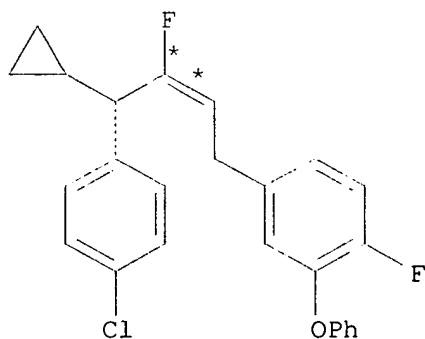


4 AD



2 BG

11
STEPS
→



AT

RX(3) RCT G 119544-56-8
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0

RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h

RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days

RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h

RX(10) RCT R 398453-56-0

STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.

RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h

RX(13) RCT Y 398453-60-6

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)
RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at -78.degree. for 2 h; 50% overall yield

RX(36) RCT AJ 398464-74-9, AL 398464-76-1, BG 108-24-7
PRO AM 398453-63-9, AW 398453-77-5
CAT 1122-58-3 4-DMAP

SOL 75-09-2 CH₂Cl₂
 NTE acetylation at room temp. for 2 h in 79% overall yield

RX(16) RCT AM 398453-63-9

STAGE(1)

RGT T 1310-73-2 NaOH
 SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

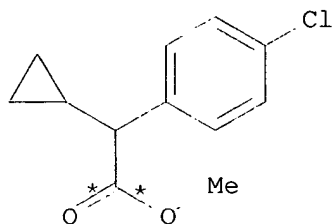
RGT U 7647-01-0 HCl
 SOL 141-78-6 AcOEt
 PRO AN 398453-70-8
 NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(20) RCT AN 398453-70-8
 RGT J 98-59-9 TsCl
 PRO AT 398453-73-1
 SOL 29611-84-5 Collidine
 NTE decarboxylation and dehydration (olefination) at 170.degree. for 2 h

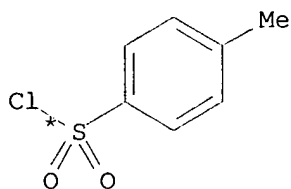
RX(398) OF 398 COMPOSED OF RX(3), RX(2), RX(5), RX(7), RX(10), RX(11), RX(13),
 RX(15), RX(37), RX(16), RX(20)

RX(398) 5 G + 4 J + 4 O + 4 V + 4 AD + 2 BG ==>

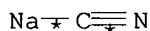
AT



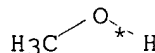
5 G



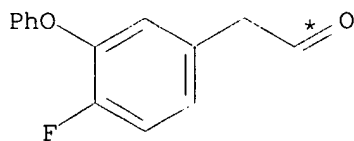
4 J



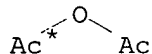
4 O



4 V

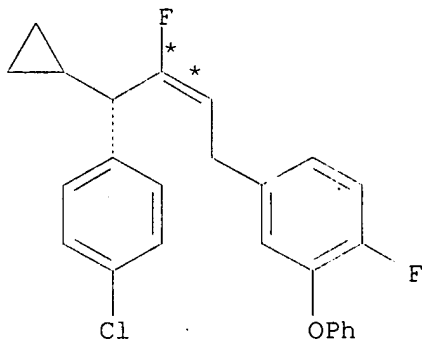


4 AD



2 BG

11
 STEPS
 —————>



AT

- RX(3) RCT G 119544-56-8
PRO A 398453-51-5, E 398453-52-6
CAT 9016-18-6 Carbonic esterase
SOL 7732-18-5 Water
NTE biotransformation; enzymic stereoselective hydrolysis at room temp. and pH 7.1-8.0
- RX(2) RCT E 398453-52-6
RGT C 14044-65-6 BH3-THF
PRO F 119544-60-4
SOL 109-99-9 THF
NTE redn. at room temp. for 4 h
- RX(5) RCT F 119544-60-4, J 98-59-9
RGT L 121-44-8 Et3N
PRO N 398453-54-8
SOL 75-09-2 CH2Cl2
NTE tosylation at room temp. for 3 days
- RX(7) RCT N 398453-54-8, O 143-33-9
PRO R 398453-56-0
SOL 67-68-5 DMSO
NTE cyanation at 90.degree. for 3 h
- RX(10) RCT R 398453-56-0
- STAGE(1)
RGT T 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
- STAGE(2)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO X 398453-58-2
NTE alkali hydrolysis under reflux for 18 h; acidification at 0.degree.
- RX(11) RCT X 398453-58-2, V 67-56-1
PRO Y 398453-60-6
CAT 7647-01-0 HCl
NTE esterification at room temp. for 18 h
- RX(13) RCT Y 398453-60-6

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RGT AB 133745-75-2 (PhSO2)NF
PRO AC 398453-62-8
NTE deprotonation at -78.degree. to 0.degree. over 5 min;
fluorination at room temp. for 2 h

RX(15) RCT AC 398453-62-8

STAGE(1)

RGT AA 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)

RCT AD 117252-07-0
PRO AI 398464-73-8, AJ 398464-74-9, AK 398464-75-0, AL 398464-76-1
NTE deprotonation at -78.degree. for 15 min; addn. reaction at
-78.degree. for 2 h; 50% overall yield

RX(37) RCT AK 398464-75-0, AJ 398464-74-9, BG 108-24-7
PRO AM 398453-63-9, AY 398453-78-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
NTE acetylation at room temp. for 2 h

RX(16) RCT AM 398453-63-9

STAGE(1)

RGT T 1310-73-2 NaOH
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

RGT U 7647-01-0 HCl
SOL 141-78-6 AcOEt
PRO AN 398453-70-8
NTE sapon. under reflux for 1 h; acidification with concd. HCl

RX(20) RCT AN 398453-70-8
RGT J 98-59-9 TsCl
PRO AT 398453-73-1
SOL 29611-84-5 Collidine
NTE decarboxylation and dehydration (olefination) at 170.degree. for
2 h

=> fil reg; d stat que 128; fil cap1; d que nos 129; fil uspatf; d que nos 130
FILE 'REGISTRY' ENTERED AT 12:00:19 ON 28 JAN 2003
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STRUCTURE FILE UPDATES: 27 JAN 2003 HIGHEST RN 482277-90-7
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TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

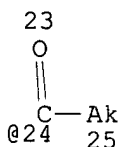
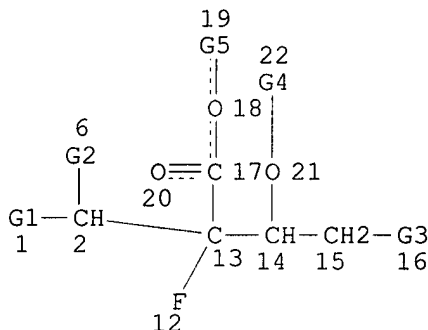
Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

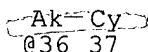
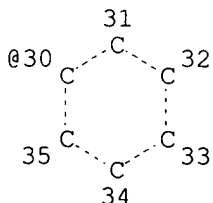
Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

L26

STR



Ak @26 Ak-X
 @27 28



*definition for Ar, (G3) expanded
as previously noted*

VAR G1=30/HY
VAR G2=26/27/CB
VAR G3=30/HY/36 }
VAR G4=H/24
VAR G5=H/26

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 25
CONNECT IS E1 RC AT 26
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

~~L28~~ 25 SEA FILE=REGISTRY SSS FUL L26

100.0% PROCESSED 1162 ITERATIONS

SEARCH TIME: 00.00.01

25 ANSWERS

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FILE COVERS 1907 - 28 Jan 2003 VOL 138 ISS 5

FILE LAST UPDATED: 27 Jan 2003 (20030127/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L26 STR
L28 25 SEA FILE=REGISTRY SSS FUL L26
~~L29~~ 1 SEA FILE=CAPLUS ABB=ON L28

FILE 'USPATFULL' ENTERED AT 12:00:19 ON 28 JAN 2003

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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 28 Jan 2003 (20030128/PD)

FILE LAST UPDATED: 28 Jan 2003 (20030128/ED)

HIGHEST GRANTED PATENT NUMBER: US6513163

HIGHEST APPLICATION PUBLICATION NUMBER: US2003019004

CA INDEXING IS CURRENT THROUGH 28 Jan 2003 (20030128/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 28 Jan 2003 (20030128/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2002

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2002

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>>> published document but also a list of any subsequent <<<
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>>> publication date for all the US publications for an invention <<<
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>>> classifications, or claims, that may potentially change from <<<
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L26 STR
L28 25 SEA FILE=REGISTRY SSS FUL L26
~~L30 1 SEA FILE=USPATFULL ABB=ON L28~~

=> dup rem 129,130

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PROCESSING COMPLETED FOR L30

~~L32 2 DUP REM L29 L30 (0 DUPLICATES REMOVED)~~
ANSWER '1' FROM FILE CAPLUS
ANSWER '2' FROM FILE USPATFULL

=> d ibib abs hitstr 1-2; fil cao; d que nos 131

L32 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:122926 CAPLUS
DOCUMENT NUMBER: 136:183615
TITLE: Process for the preparation of chiral insecticidal and acaricidal 1,4-diaryl-2-fluoro-2-butenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid methyl ester using esterase
INVENTOR(S): Chiarello, John Francis; Buckwalter, Brian Lee; Barden, Timothy Claude
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012155	A2	20020214	WO 2001-EP9012	20010803
WO 2002012155	A3	20021128		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002032351 A1 20020314 US 2001-921188 20010802

AU 2001082067 A5 20020218 AU 2001-82067 20010803

PRIORITY APPLN. INFO.:

US 2000-222733P P 20000803

WO 2001-EP9012 W 20010803

OTHER SOURCE(S): CASREACT 136:183615; MARPAT 136:183615

AB There is provided a process for the prepn. of a chiral compd. of formula $\text{ArC}^*\text{H(R)CF:CHAr1}$ [I; Ar, Ar1 = (un)substituted aryl or a 5- or 6-membered heteroarom. ring; R is C1-4 alkyl, C1-4 haloalkyl, C3-6 cycloalkyl or C3-6 halocycloalkyl; Ar1, is aryl or a 5- or 6-membered heteroarom. ring; C* represents an asym. center] which is useful as an insecticidal and acaricidal agent and for protecting plants from damage caused by insect and acarid attack and infestation (no data). Also provided are intermediate compds. useful in the process of the present invention. This process comprises (a) treating a racemic ester of formula $\text{ArCH(R)CO}_2\text{R4}$ (II; Ar, R = same as above; R4 = C1-4 alkyl) with an esterase to form a first mixt. of either R-acid of formula $\text{ArCH(R)CO}_2\text{H}$ (III) and S-ester of formula II or of S-acid of formula III and R-ester of formula II, (b) sepg. (R)- or (S)-acid III from said (S)- or (R)-ester II, (c) reducing the chiral acid (R)- or (S)-acid III or (S)- or (R)-ester II to obtain a chiral alc. of formula (R)- or (S)- $\text{ArC}^*\text{H(R)CH}_2\text{OH}$, (d) transforming the chiral alc. into an ester (R)- or (S)- $\text{ArC}^*\text{H(R)CH}_2\text{CO}_2\text{R1}$, (e) fluorinating the latter ester to afford a fluoro-ester (R)- or (S)- $\text{ArC}^*\text{H(R)CHFCO}_2\text{R1}$, and (f) reacting the latter fluoro-ester with an aldehyde $\text{Ar1CH}_2\text{CHO}$ (Ar1 = same as above) in a solvent in the presence of a base to afford a second mixt. of 4 chiral diastereomeric hydroxy-esters $\text{ArC}^*\text{H(R)CHF(CO}_2\text{R1)CH(OH)CH}_2\text{Ar1}$. It further comprises (g) optionally sepg. the second mixt. into a third mixt. each having two chiral diastereomers, (h) treating the hydroxy-ester mixts. with an acylating agent $\text{R}_2\text{COX1}$ (R_2 = C1-4 alkyl; X1 = Cl, Br, R_2CO_2) to afford a fifth mixt. of 4 chiral diastereomeric acyloxy esters or a seventh mixt. of two chiral diastereomeric acyloxy esters $\text{ArC}^*\text{H(R)CHF(CO}_2\text{R1)CH(O}_2\text{CR}_2\text{)CH}_2\text{Ar1}$, (i) optionally sepg. the sixth or seventh mixt. not essentially pure chiral diastereomeric acyloxy ester, (j) hydrolyzing the pure acyloxy esters or mixts. of esters to afford a hydroxy acid $\text{ArC}^*\text{H(R)CHF(CO}_2\text{H)CH(OH)CH}_2\text{Ar1}$, and (k) heating the hydroxy acid with a arylsulfonyl halide to afford I. Thus, Me (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate was treated with horse liver esterase in water (pH 7.5) to give 37.9% (2R)-(4-chlorophenyl)(cyclopropyl)ethanoic acid and 36.2% Me (2S)-(4-chlorophenyl)(cyclopropyl)ethanoate, each of which was reduced by $\text{BH}_3\cdot\text{THF/THF}$ at room temp. for 4 h and DIBAL/ CH_2Cl_2 warming from -78.degree. to room temp. and at room temp. for 1 h, resp., to give 84% (2R)-(4-chlorophenyl)(cyclopropyl)ethanol and 80% (2S)-(4-chlorophenyl)(cyclopropyl)ethanol, resp. Each of (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethanol was tosylated by tosyl chloride in the presence of Et3N in CH_2Cl_2 to (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethyl p-toluenesulfonate, resp., which underwent cyanation with NaCN in DMSO at 90.degree. for 3 h to give (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile, resp. Alkali hydrolysis of (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile in a mixt. of 10% aq. NaOH and methanol under reflux for 18 h followed by acidification with concd. HCl gave (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoic acid, resp., which was esterified with MeOH in the presence of HCl at room temp. for 18 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate, resp. Lithiation of the each ester with lithium diisopropylamide (LDA) in THF at -78.degree. to 0.degree. followed by fluorination with $(\text{PhSO}_2)_2\text{NF}$ at -78.degree. to room temp. and room temp. for 2 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate, resp. Lithiation of Me (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate with LDA in THF at -78.degree. for 15 min followed by addn. reaction with 4-fluoro-3-phenoxyphenylacetaldehyde at -78.degree. for 2 h gave, after

silica gel chromatog., an oil (A) contg. (2R,3R) and (2R,3S) or (2S,3R)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate and an oil contg. (2S,3S) and (2S,3R) or (2R,3S)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate (steps f and g). Acetylation of the oil A with Ac2O in the presence of DAMP in CH2Cl2 at room temp. for 2 h gave Me (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate and Me (2R,3S or 2S,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate (step h and i). Alkali hydrolysis of the latter diastereomer in a mixt. of 10% aq. NaOH, MeOH, and THF under reflux for 1 h gave (2S,3R or 2R,3S)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid (step j) which was heated with tosyl chloride in collidine at 170.degree. for 2 h to give 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene as a colorless oil (step k).

IT **398453-63-9P**, Methyl (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-64-0P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-66-2P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-67-3P**, Methyl (2R,3R)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-68-4P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-69-5P**, (2S,3S)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-70-8P**, (2R,3R)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-71-9P**, (2R,3R)-2-[(R)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-76-4P** **398453-77-5P**, Methyl (2R,3S)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-78-6P** **398453-79-7P** **398453-80-0P** **398453-81-1P** **398453-82-2P** **398453-83-3P** **398453-84-4P** **398464-67-0P** **398464-69-2P** **398464-70-5P** **398464-71-6P** **398464-73-8P** **398464-74-9P** **398464-75-0P** **398464-76-1P**

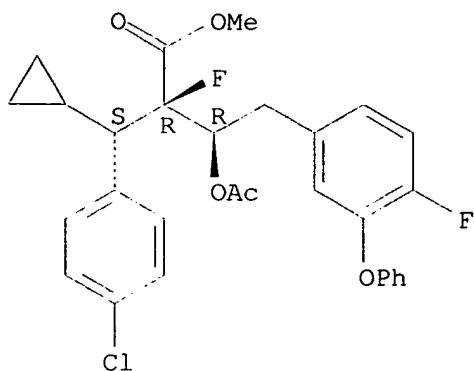
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

RN **398453-63-9** CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

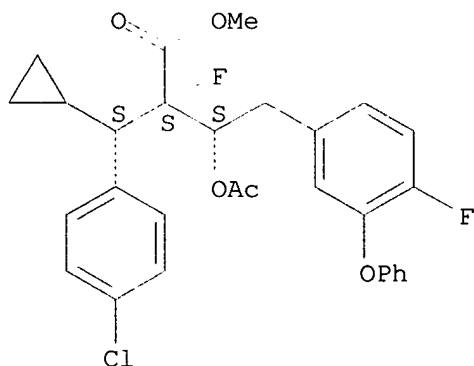
Absolute stereochemistry.



RN 398453-64-0 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

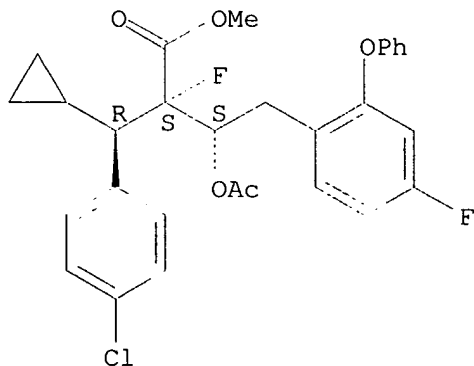
Absolute stereochemistry.



RN 398453-66-2 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-2-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

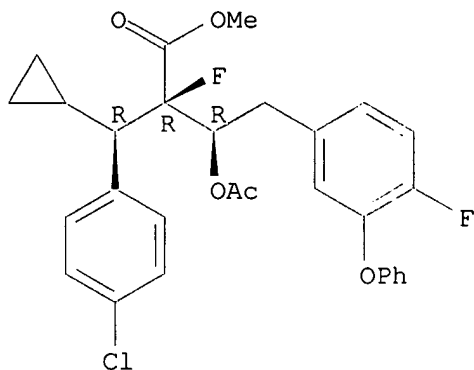


RN 398453-67-3 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

ester, (.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

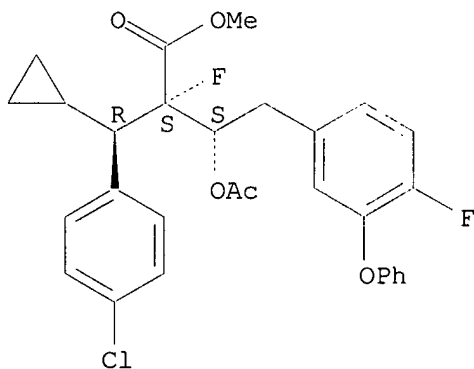
Absolute stereochemistry.



RN 398453-68-4 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

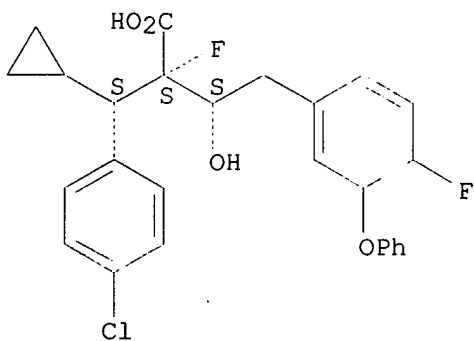
Absolute stereochemistry.



RN 398453-69-5 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

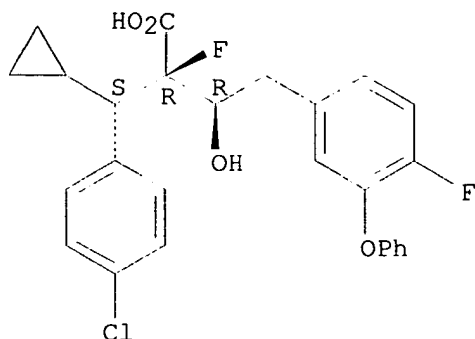
Absolute stereochemistry.



RN 398453-70-8 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.R)- (9CI)
(CA INDEX NAME)

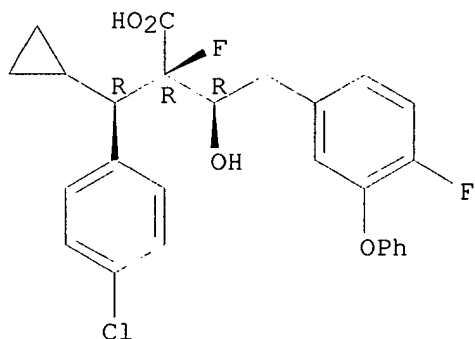
Absolute stereochemistry.



RN 398453-71-9 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.R)- (9CI)
(CA INDEX NAME)

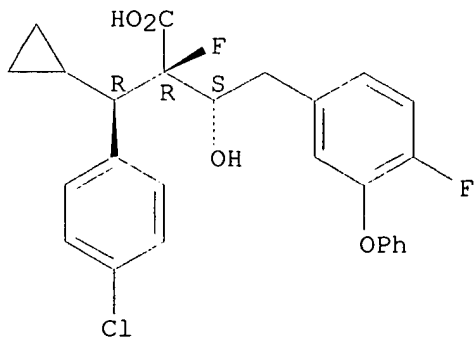
Absolute stereochemistry.



RN 398453-76-4 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.S)- (9CI)
(CA INDEX NAME)

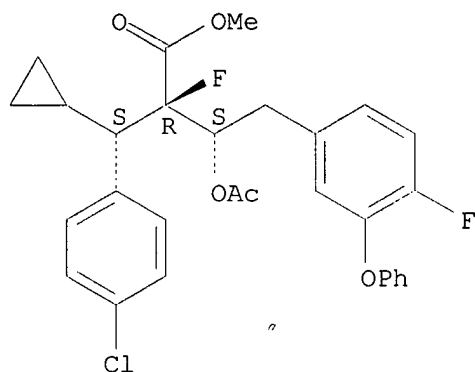
Absolute stereochemistry.



RN 398453-77-5 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

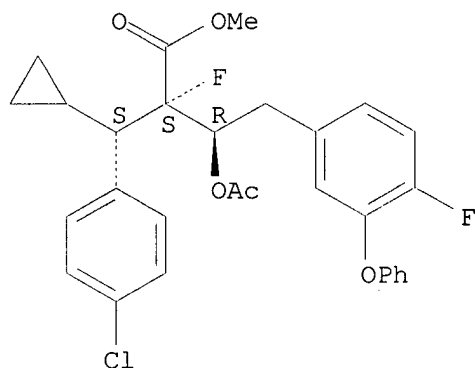
Absolute stereochemistry.



RN 398453-78-6 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

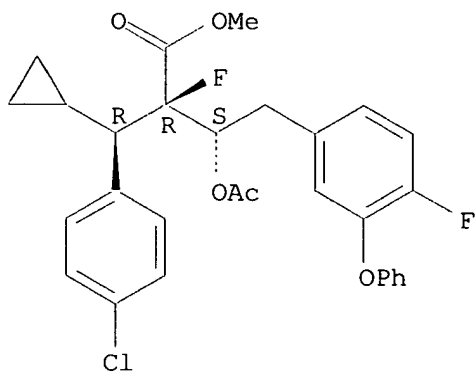
Absolute stereochemistry.



RN 398453-79-7 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

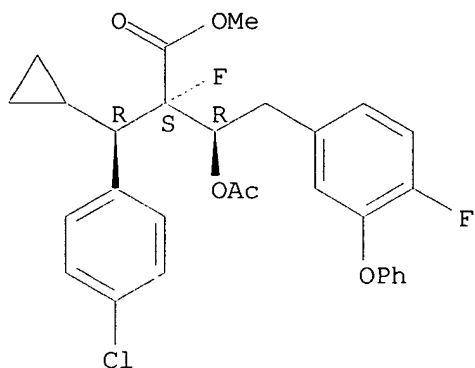
Absolute stereochemistry.



RN 398453-80-0 CAPLUS

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

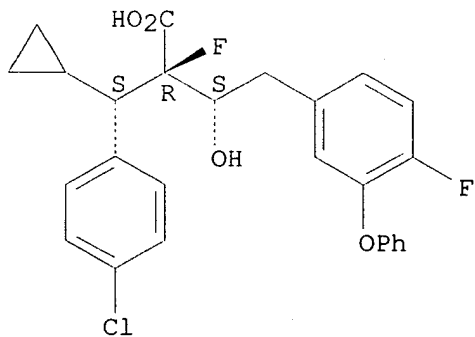
Absolute stereochemistry.



RN 398453-81-1 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

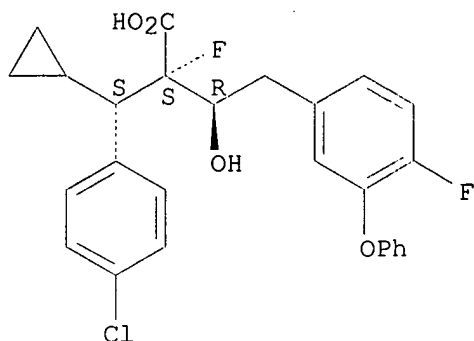
Absolute stereochemistry.



RN 398453-82-2 CAPLUS

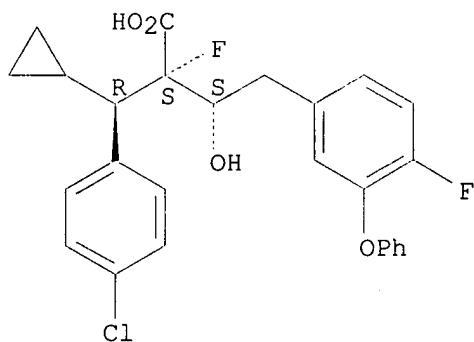
CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



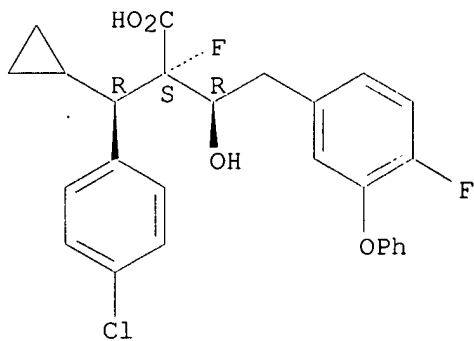
RN 398453-83-3 CAPLUS
 CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
 .alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



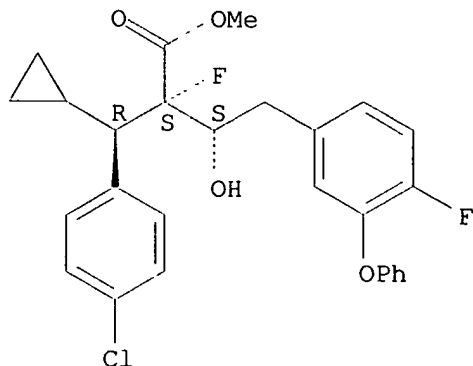
RN 398453-84-4 CAPLUS
 CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
 .alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.R)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 398464-67-0 CAPLUS
 CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
 .alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
 (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

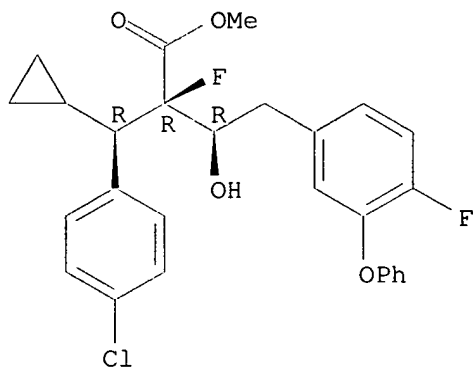
Absolute stereochemistry.



RN 398464-69-2 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

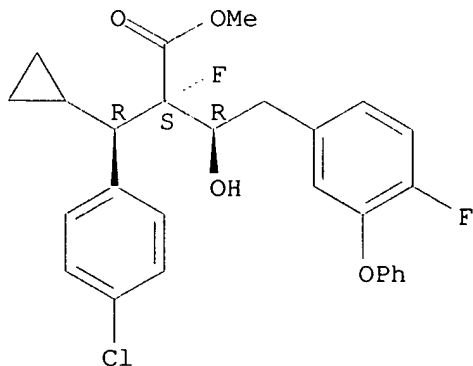
Absolute stereochemistry.



RN 398464-70-5 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

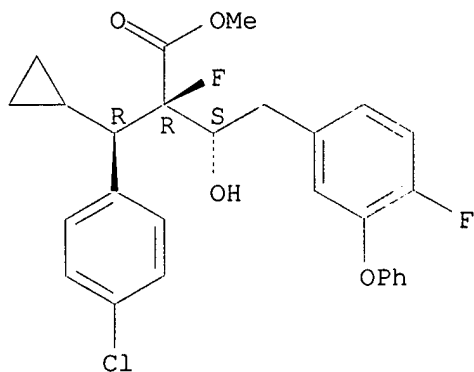
Absolute stereochemistry.



RN 398464-71-6 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

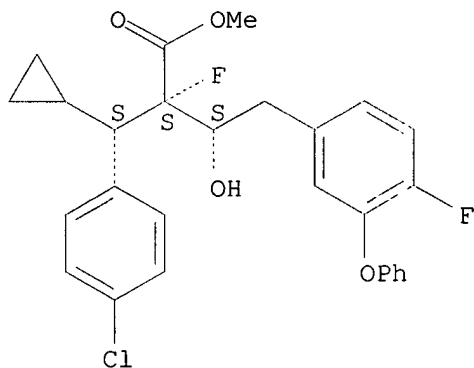
Absolute stereochemistry.



RN 398464-73-8 CAPLUS

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

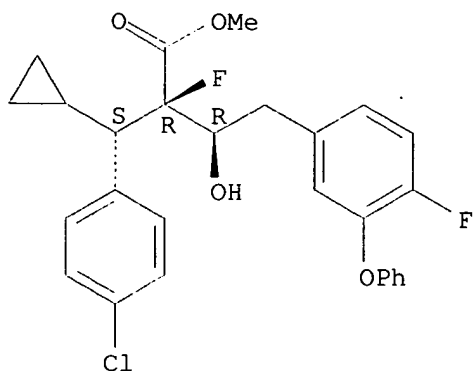
Absolute stereochemistry.



RN 398464-74-9 CAPLUS

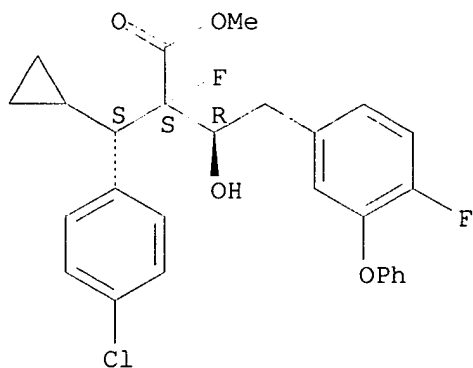
CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



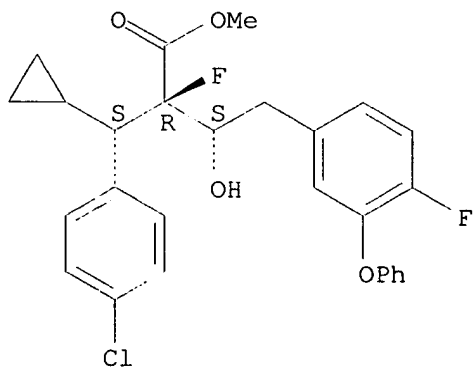
RN 398464-75-0 CAPLUS
CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 398464-76-1 CAPLUS
CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 2 OF 2 USPATFULL
ACCESSION NUMBER: 2002:55187 USPATFULL

TITLE: Process for the preparation of chiral isofluoroenes
INVENTOR(S): Chiarello, John Francis, Newtown, PA, UNITED STATES
Buckwalter, Brian Lee, Yardley, PA, UNITED STATES
Barden, Timothy Claude, Holland, PA, UNITED STATES
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Ludwigshafen, GERMANY, FEDERAL
REPUBLIC OF (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002032351	A1	20020314
APPLICATION INFO.:	US 2001-921188	A1	20010802 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-222733P	20000803 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	Susan Shaw, Intellectual Property Department, BASF Corporation, 3000 Continental Drive - North, Mount Olive, NJ, 07828-1234	
NUMBER OF CLAIMS:	11	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1076	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB There is provided a process for the preparation of a chiral insecticidal and acaricidal compound of formula I. ##STR1##

Also provided are intermediate compounds useful in the process of the present invention.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

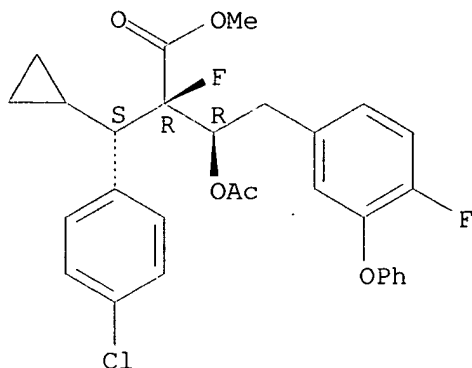
IT **398453-63-9P**, Methyl (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-64-0P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-66-2P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-2-phenoxyphenyl)butanoate **398453-67-3P**, Methyl (2R,3R)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-68-4P**, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-69-5P**, (2S,3S)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-70-8P**, (2R,3R)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-71-9P**, (2R,3R)-2-[(R)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid **398453-76-4P** **398453-77-5P**, Methyl (2R,3S)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate **398453-78-6P** **398453-79-7P** **398453-80-0P** **398453-81-1P** **398453-82-2P** **398453-83-3P** **398453-84-4P** **398464-67-0P** **398464-69-2P** **398464-70-5P** **398464-71-6P** **398464-73-8P** **398464-74-9P** **398464-75-0P** **398464-76-1P**

(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

RN 398453-63-9 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha., 4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

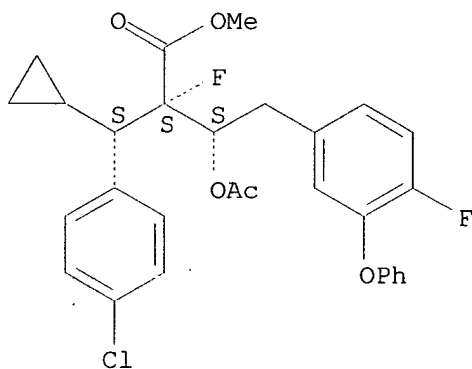
Absolute stereochemistry.



RN 398453-64-0 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

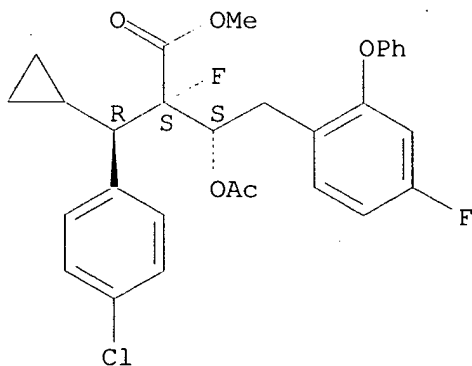
Absolute stereochemistry.



RN 398453-66-2 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-2-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

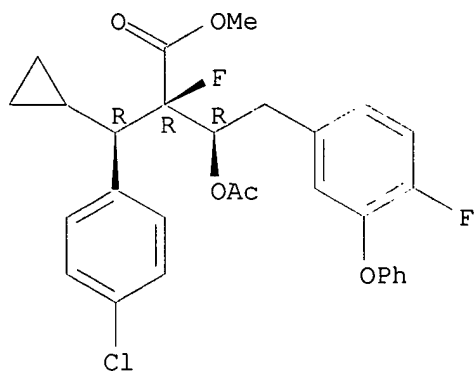
Absolute stereochemistry.



RN 398453-67-3 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

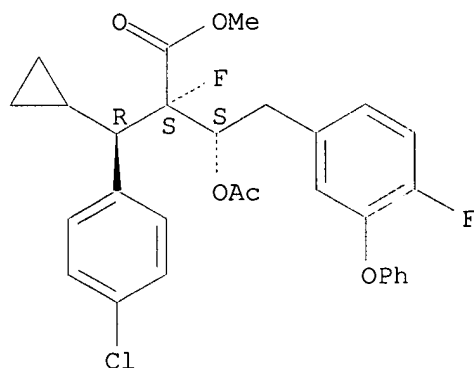
Absolute stereochemistry.



RN 398453-68-4 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

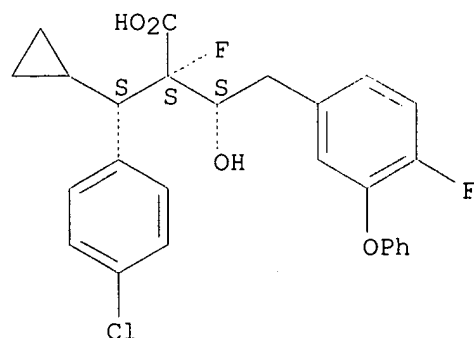
Absolute stereochemistry.



RN 398453-69-5 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

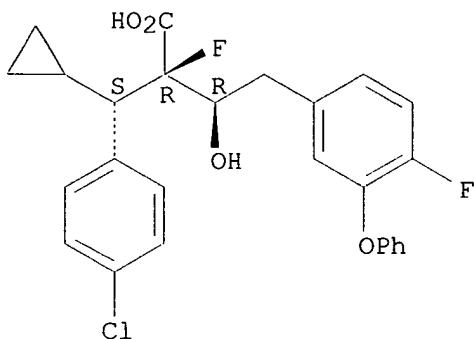
Absolute stereochemistry.



RN 398453-70-8 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.R)- (9CI)
(CA INDEX NAME)

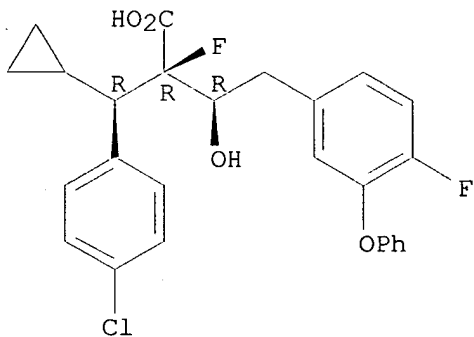
Absolute stereochemistry.



RN 398453-71-9 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.R)- (9CI)
(CA INDEX NAME)

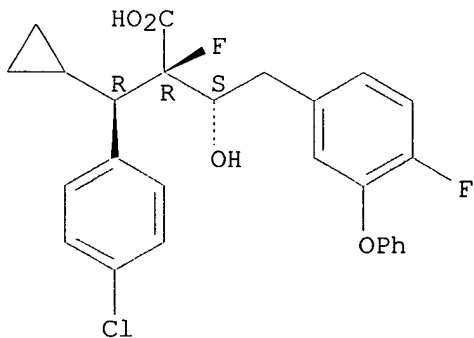
Absolute stereochemistry.



RN 398453-76-4 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.S)- (9CI)
(CA INDEX NAME)

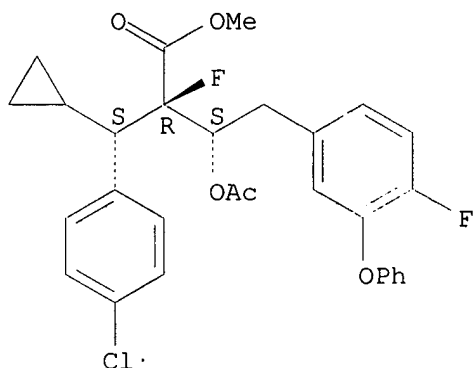
Absolute stereochemistry.



RN 398453-77-5 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

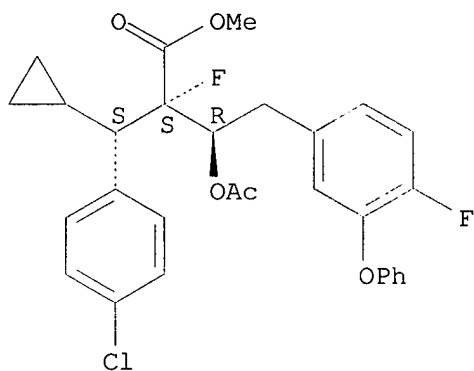
Absolute stereochemistry.



RN 398453-78-6 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

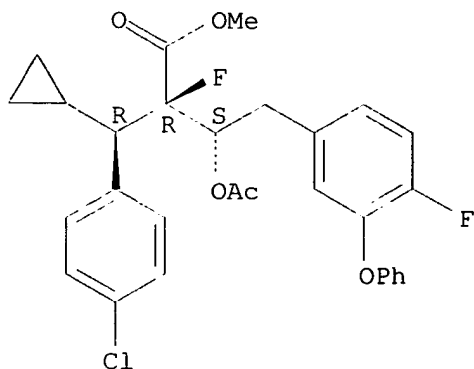
Absolute stereochemistry.



RN 398453-79-7 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

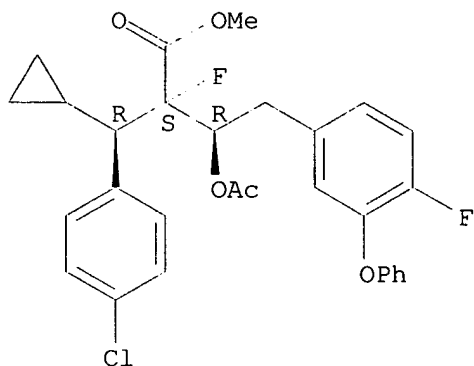
Absolute stereochemistry.



RN 398453-80-0 USPATFULL

CN Benzenebutanoic acid, .beta.-(acetyloxy)-.alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-3-phenoxy-, methyl ester, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

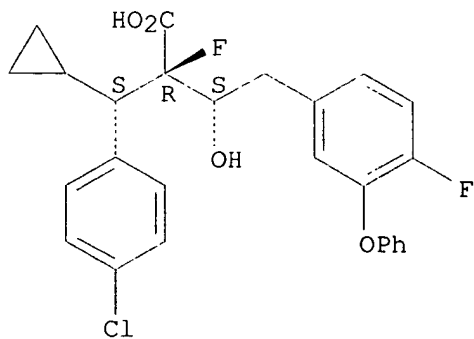
Absolute stereochemistry.



RN 398453-81-1 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

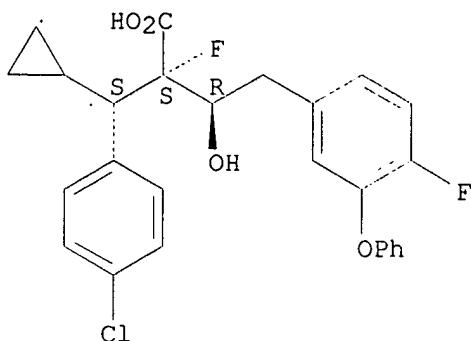
Absolute stereochemistry.



RN 398453-82-2 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

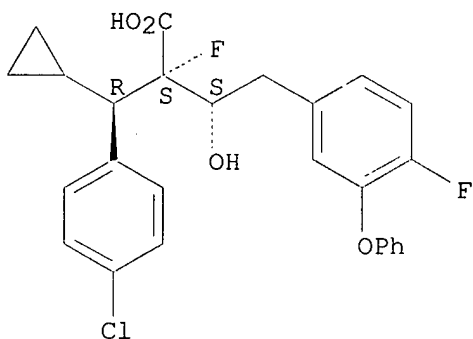
Absolute stereochemistry.



RN 398453-83-3 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.S)- (9CI)
(CA INDEX NAME)

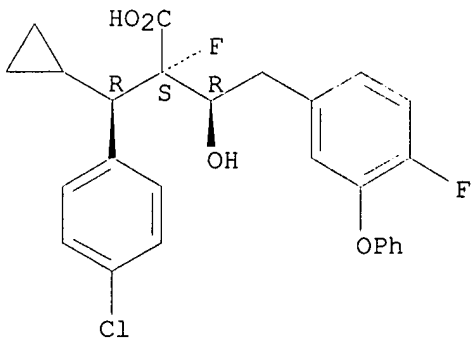
Absolute stereochemistry.



RN 398453-84-4 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, (.alpha.S,.beta.R)- (9CI)
(CA INDEX NAME)

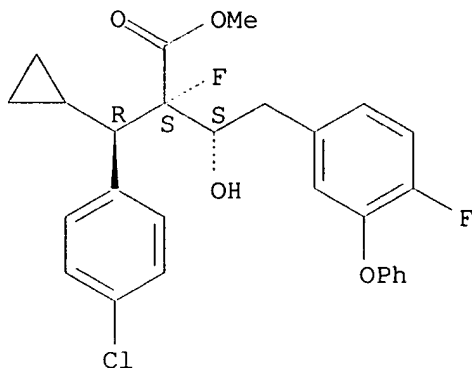
Absolute stereochemistry.



RN 398464-67-0 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

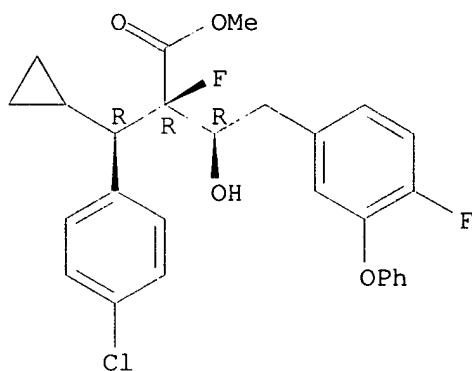
Absolute stereochemistry.



RN 398464-69-2 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

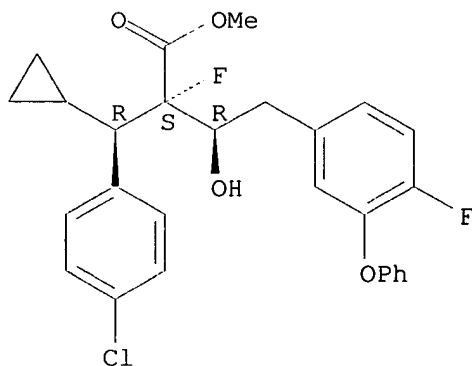
Absolute stereochemistry.



RN 398464-70-5 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

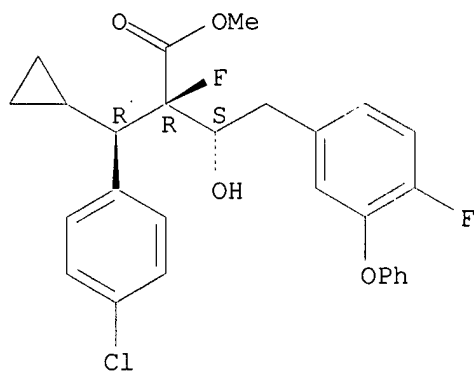
Absolute stereochemistry.



RN 398464-71-6 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(R)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

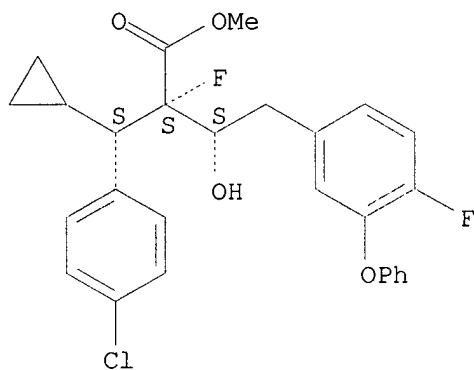
Absolute stereochemistry.



RN 398464-73-8 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.S)- (9CI) (CA INDEX NAME)

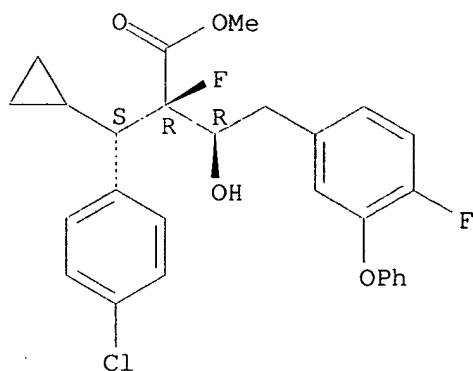
Absolute stereochemistry.



RN 398464-74-9 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.R)- (9CI) (CA INDEX NAME)

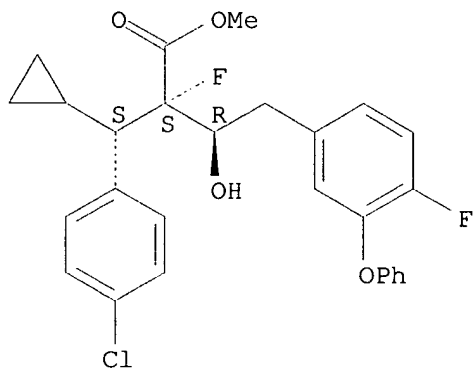
Absolute stereochemistry.



RN 398464-75-0 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.S,.beta.R)- (9CI) (CA INDEX NAME)

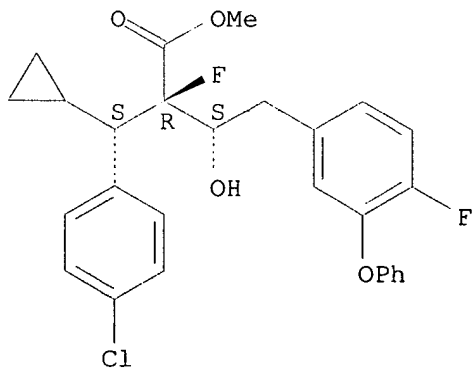
Absolute stereochemistry.



RN 398464-76-1 USPATFULL

CN Benzenebutanoic acid, .alpha.-[(S)-(4-chlorophenyl)cyclopropylmethyl]-
.alpha.,4-difluoro-.beta.-hydroxy-3-phenoxy-, methyl ester,
(.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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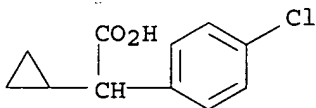
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03225

L6 ANSWER 166 OF 172 CAPLUS COPYRIGHT 2002 ACS
 AN 1970:12378 CAPLUS
 DN 72:12378
 TI .alpha.-Phenylcycloaliphatic acids and amides
 IN Dickel, Daniel F.; De Stevens, George
 PA CIBA Ltd.
 SO Ger. Offen., 51 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 1913531	A	19691009	DE 1969-1913531	19690318
	NL 6903270	A	19690930	NL 1969-3270	19690303
	FR 2004826	A1	19691205	FR 1969-8704	19690325
	BE 730523	A	19690926	BE 1969-730523	19690326
	US 3786085	A	19740115	US 1969-858893	19690917
	US 3880916	A	19750429	US 1973-350447	19730412
PRAI	US 1968-716290		19680327		
	US 1969-789076		19690102		
	US 1969-808341		19690318		
	US 1969-858893		19690917		
IT	24438-45-7P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	24438-45-7 CAPLUS				
CN	Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)				



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921188

L6 ANSWER 162 OF 172 CAPLUS COPYRIGHT 2002 ACS
AN 1978:50521 CAPLUS
DN 88:50521
TI Insecticidal cyclopropylphenylacetic acid esters
IN Elliott, Michael; Janes, Norman Frank; Pulman, David Allen
PA National Research Development Corp., UK
SO Ger. Offen., 26 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN. CNT 1

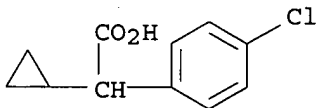
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2717414	A1	19771103	DE 1977-2717414	19770420
	DE 2717414	C2	19871015		
	GB 1580193	A	19801126	GB 1976-16234	19760422
	NL 7704252	A	19771025	NL 1977-4252	19770419
	US 4137324	A	19790130	US 1977-789226	19770420
	JP 52131563	A2	19771104	JP 1977-46689	19770421
	JP 62029422	B4	19870625		
	FR 2348919	A1	19771118	FR 1977-12082	19770421
	FR 2348919	B1	19820716		
PRAI	GB 1976-16234		19760422		

IT 24438-45-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)

RN 24438-45-7 CAPLUS

CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



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